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A COMPUTER MODEL FOR PREDICTING LEAK RATES OF CHEMICALS FROM DAMAGED STORAGE AND TRANSPORTATION TANKS

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A COMPUTER MODEL FOR PREDICTING LEAK RATES OF CHEMICALS FROM DAMAGED STORAGE AND TRANSPORTATION TANKS

by

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ABSTRACT

A computer model has been developed to predict the outflow rate and duration of leaks from damaged chemical storage and transportation tanks. The model is simple to use and requires no knowledge of chemical properties beyond name and the mass in the tank. The model predicts chemical properties, outflow rates, tank temperatures and spill duration for ammonia, benzene, chlorine and hydrogen sulphide. Example leak nomographs are provided for these chemicals for ruptures above and below the liquid level in a standard rail tank car. Major differences between the EnviroTIPS nomographs and the computer model are noted for the case of liquified gas tanks with ruptures in the vapour space.

Recommendations arising from the project include a small or meso-scale test program to validate the model and the inclusion of more chemicals.

FOREWORD

This study was conducted by Mr. I.A. Buist and Mr. R.C. Belore of S.L. Ross Environmental Research Limited, under contract to the Environmental Protection Service. Mr. M.F. Fingas of the Environmental Emergencies Technology Division was the Scientific Authority.

TABLE OF CONTENTS

	Page
ABSTRACT	i
RESUME	ii
FOREWORD	iii
LIST OF FIGURES	vii
LIST OF TABLES	viii
1.0 INTRODUCTION	1
2.0 DESCRIPTION OF MODEL	3
2.1 Chemical Selection	4
2.2 Environmental Data	4
2.3 Tank Specifications	6
2.4 Rupture Specifications	6
2.5 Chemical Properties	9
2.5.1 Gaseous State	9
2.5.1.1 Gas Density	9
2.5.1.2 Gas Heat Capacity & Ratio	9
2.5.2 Liquid State	11
2.5.2.1 Liquid Density	11
2.5.2.2 Liquid Heat Capacity	12
2.5.2.3 Heat of Vaporization	12
2.5.2.4 Surface Tension	12
2.5.2.5 Kinematic Viscosity Ratio	13
2.5.2.6 Vapour Pressure	13

TABLE OF CONTENTS

		Page
2.6	Gas Flow Through Rupture	13
2.6.1	Sonic Flow	14
2.6.2	Subsonic Flow	15
2.7	Liquid Flow Through Rupture	15
2.7.1	Air Ingestion	16
2.7.2	Evaporation Losses	16
2.8	Two-Phase Flow Through Rupture	17
2.8.1	Void Fraction	17
2.8.2	Hole Below Liquid Level	19
2.8.2.1	Two-Phase Subsonic Flow	19
2.8.2.2	Two-Phase Sonic Flow	19
2.8.3	Hole in Vapour Space	20
2.9	Heat Transfer	21
2.9.1	Overall Heat Transfer Coefficient	22
2.9.2	Outside Heat Transfer Coefficient	22
2.9.3	Inside Heat Transfer Coefficient	23
2.9.4	Insulation Losses	24
3.0	COMPUTER PROGRAM DESIGN	25
3.1	Mainline Program Structure - "LEAKR"	25
3.2	Gas Discharge Model - "GASMOD"	30
3.3	Liquid Discharge Model - "LIQMOD"	31
3.4	Vapour Release Model - "VAPMOD"	32

TABLE OF CONTENTS

		Page
4.0	MODEL RESULTS	34
5.0	CONCLUSIONS AND RECOMMENDATIONS	43
	5.1 Conclusions	43
	5.2 Recommendations	45
6.0	REFERENCES	46
	APPENDIX I - COMPUTER PROGRAM LISTING	

LIST OF FIGURES

Figure		Page
1.	Mainline Program Structure	26
2.	Gas Discharge Model Structure	27
3.	Liquid Discharge Model Structure	28
4.	Vapour Discharge Model Structure	29
5.	Benzene Discharge Nomograph - hole in bottom of tank car	36
6.	Chlorine Discharge Nomograph - hole in bottom of tank car	37
7.	Chlorine Discharge Nomograph - hole in top of tank car	38
8.	Ammonia Discharge Nomograph - hole in bottom of tank car	39
9.	Ammonia Discharge Nomograph - hole in top of tank car	40
10.	Hydrogen Sulphide Discharge Nomograph - hole in bottom of tank car	41
11.	Hydrogen Sulphide Discharge Nomograph - hole in top of tank car	42

LIST OF TABLES

Table		Page
1.	Critical Constants for Selected Chemicals	5
2.	Tank Geometry Formulae	7
3.	Discharge Coefficients for Liquid or Two-Phase Flow	8
4.	Outside Heat Transfer Coefficient Constants	23

1.0 INTRODUCTION

A simple, yet accurate technique is needed to predict the rate at which chemicals (liquid or gaseous) leak from damaged storage or transportation containers. Accurate predictions of the outflow rate and duration of the incident are vital for the planning of a safe and effective emergency response. Of particular importance to the response effort is the "source strength" component of the release. This source term is required by all atmospheric dispersion models which predict the areas which should be evacuated due to the release of the hazardous chemical.

Nomograms for predicting these chemical leak rates and durations were developed for the EnviroTIPS series of manuals (Environment Canada, 1983). Unfortunately many simplifications were made in the development of these nomograms in order to make them easy to use. For example, a number of assumptions were made to force the prediction of a maximum rate of release. This may or may not represent a "worst-case situation" for some accidents. A slow emission rate for a very toxic substance may necessitate the evacuation of a large area for the entire leak period. A model which is forced to generate maximum release rates falsely predicts a much shorter hazard period.

The objective of this study was to improve the existing nomograms by using more rigorous assumptions and equations for the transfer processes involved (heat, fluid and mass). The system of equations was used to develop a model on a micro-computer (IBM-PC) to permit rapid solution of the iterative balance equations and thus reduce the number of simplifying (and often misleading) assumptions required. Only five representative chemicals are presently included in the model, though others can be easily added.

Section 2.0 of this report describes the equations used and the structure of the model. Section 3.0 describes the computer program and Section 4.0 gives examples of the model outputs for various spill scenarios and compares these with the EnviroTIPS nomograph predictions. Section 5.0 presents the conclusions and recommendations arising from the study. A complete computer program listing is given in the Appendix.

2.0 DESCRIPTION OF MODEL

In order to more fully approximate the real physical situation existing after the rupture of a storage or transportation tank containing chemicals, several sub-models were developed and then linked in the computer program. These sub-models include:

* a menu driven routine to select the spilled chemical and specify the seven parameters necessary to fully describe its physical, chemical and thermodynamic properties over the ranges of pressure and temperature,

* an input program to read in the various environmental parameters required,

* a menu driven program to select the type of tank involved and its orientation and calculate the geometric relationships between volume, height of liquid/vapour and heat transfer area

* a menu driven program to select the type, location and orientation of the rupture and to specify the fluid dynamics of the rupture

* a physical/chemical/thermodynamic properties model to calculate, based on the chemical selected and the environmental conditions, the required properties for the heat transfer, mass transfer and fluid dynamics models

* three rupture fluid discharge models, one to describe the release of a compressed gas, one to describe the release of liquid from a hole (including two-phase flow) and one to describe the release of vapour from a rupture above a boiling liquid

* a heat transfer model to calculate the temperature of the tank contents as a function of environmental conditions, tank properties and rate of evaporation of the liquid phase

* three mass balance models; one to calculate pressure drops for leaks in gas tanks, one to predict two-phase flow qualities and one to predict evaporation rates under depressurization conditions

The components of each of these sub-models is described below. The linking of the sub-models to form the computer program is described at the end of this section.

2.1 CHEMICAL SELECTION

The model contains five specified chemicals representative of those normally stored and transported in Canada. These are; chlorine, benzene, hydrogen sulphide, anhydrous ammonia and sulphuric acid (66^{o} Be).

The values of the seven parameters which are sufficient to fully describe the physical, chemical and thermodynamic properties of each of the chemicals are stored in this routine. A list of these parameters is given in Table 1.

2.2 ENVIRONMENTAL DATA

The following environmental data are required for the various sub-models:

* T_{air} - air temperature (^{o}K)
* P_{atm} - atmospheric pressure (N/m^2)
* U_{wind} - wind speed (m/s)

TABLE 1

CRITICAL CONSTANTS FOR SELECT CHEMICALS

CHEMICAL	BOILING POINT (^{o}K)	CRITICAL TEMPERATURE (^{o}K)	CRITICAL PRESSURE (N/m^2)	MOLECULAR WEIGHT	A*	B* ($x10^3$)	C* ($x10^6$)
CHLORINE	238.4	417	77.1×10^5	70.91	7.576	2.424	-0.965
BENZENE	353.1	561.5	48.3×10^5	78.11	-0.409	77.621	-26.429
HYDROGEN SULPHIDE	213.4	373.4	90.1×10^5	34.08	6.662	5.134	-0.854
AMMONIA	239.6	405.4	113.0×10^5	17.03	6.086	8.812	-1.506
SULPHURIC ACID	563	N/A+	N/A	116.09	N/A	N/A	N/A

* constants required to calculate heat capacity of gases or vapours

\+ not available

2.3 TANK SPECIFICATIONS

In order that the model be as flexible as possible, a wide range of tank sizes, orientations and insulation may be specified. From this and a calculation of the initial height of the liquid (or pressure in the case of a compressed gas), the relationship between outflow rate, liquid level (or pressure for a gas), amount of chemical remaining and heat transfer area can be determined and calculated. Four basic tank types can be specified, rectangular, spherical, or cylindrical (oriented either vertically or horizontally). The dimensional relationships for each of these tank types is given in Table 2. Tank wall thickness, insulation thickness and insulation losses are also input here.

2.4 RUPTURE SPECIFICATIONS

The rupture in the tank is defined by a shape (circular or rectangular), dimensions, orientation (horizontal or vertical), edge condition (smooth, uniform petals jagged in or out, random petals jagged in), and location (vertical distance from tank bottom to rupture centreline). The coefficient of discharge for liquid or two phase flow through each type of rupture has been taken from Dodge et al, 1980. The values are shown in Table 3. For gas or vapour flow the discharge coefficient is set at 0.61.

TABLE 2

TANK GEOMETRY FORMULAE

TANK TYPE	TANK VOLUME, V_T (m^3)	LIQUID VOLUME, V_L (m^3)	HEAT TRANSFER AREA A_{SA} (m^2)	LIQUID/VAPOUR INTERFACIAL AREA A_{SC} (m^2)	HEIGHT OF LIQUID h_L (m)
RECTANGULAR	LWh_T	LWh_L	$2LH_L + 2hW + LW$	LW	V_L/LW
SPHERICAL	$\frac{4}{3}\pi r^3$	$\frac{\pi}{3} h_L{}^2(3r-h_L)$	$2\pi(2r^2-rd)$	$\pi(2rh_L-h_L^2)$	iterative solution
CYLINDRICAL					
-VERTICAL	$\pi r^2 h_t$	$\pi r^2 h_L$	$\pi(2rh_L + r^2)$	πr^2	$V_L/\pi r^2$
-HORIZONTAL	$\pi r^2 L$	$\frac{Lr^2}{2}(\Theta - \sin\Theta)$	$2\pi(rL + r^2)$	$2L(2rh_L - h_L^2)^{1/2}$	iterative solution

where L = horizontal length of tank (m)

h_T = vertical height of tank (m)

W = width of tank (m)

r = radius of tank (m)

d = depth of penetration of spherical tank into ground (m)

$\Theta = 2\cos^{-1}(1-h_L/r)$

TABLE 3

DISCHARGE COEFFICIENTS FOR LIQUID OR TWO-PHASE FLOW

RUPTURE SHAPE	EDGE* CONDITION	ORIENTATION	DISCHARGE COEFFICIENT
Circular	Smooth	---	0.65
Circular	UPJI	---	0.622
Circular	RPJI	---	0.577
Rectangular	Smooth	Horizontal	0.619
Rectangular	Smooth	Vertical	0.625
Rectangular	UPJI	Horizontal	0.629
Rectangular	UPJI	Vertical	0.626
Rectangular	RPJI	Horizontal	0.609
Rectangular	RPJI	Vertical	0.613
Rectangular	UPJO	Horizontal	0.826
Rectangular	UPJO	Vertical	0.828

* UPJI = Uniform Petals Jagged In
UPJO = Uniform Petals Jagged Out
RPJI = Random Petals Jagged In

source: Dodge et al, 1980

2.5 CHEMICAL PROPERTIES

2.5.1 Gaseous State

The basis for the calculation of the chemical properties for the gaseous state is the Redlich-Kwong equation of state (Redlich & Kwong, 1949):

$$P\underline{V} = ZRT \tag{1}$$

$$Z = (1/1-[b/\underline{V}])-(a/RT^{3/2}\underline{V}[1+(b/\underline{V})]) \tag{2}$$

and

$$a = 0.4278\ R^2T_C^{5/2} \tag{3}$$

$$b = 0.0867\ RT_C/P_C \tag{4}$$

where P = pressure (N/m^2)
$\underline{V}$ = molar volume (m^3/kg mole)
Z = compressibility factor
R = 8.314×10^3 (J/kg mole ^oK)
T = temperature (^oK)
T_C = critical temperature (^oK)

2.5.1.1 Gas Density

The gas (or vapour) density is calculated using an iterative procedure. Given an initial pressure and temperature an initial guess of molar volume is calculated from:

$$\underline{V}_i = RT/P \tag{5}$$

The value of Z is then calculated using equations 2, 3 and 4 and the next value of molar volume is calculated by:

$$\underline{V}_{i+1} = Z\ RT/P \tag{6}$$

The process is repeated until two consecutive values of V are less than 1% apart. The vapour density is then given by:

$$\rho_V = M.W./V_{i+1} \quad (7)$$

where ρ_V = vapour density (kg/m^3)
M.W. = molecular weight of chemical (kg/kg mole)

2.5.1.2 Gas Heat Capacity and Ratio

The heat capacity at constant pressure is calculated from (Balzhizer et al, 1972);

$$C_{Pg} = 4.184 \times 10^3 (A+BT+CT^2)/M.W. \quad (8)$$

where C_{Pg} = heat capacity at constant pressure of 1 atm. ($J/kg\ ^oK$)
A,B,C, = constants for each chemical (see Table 1)

The heat capacity is adjusted for pressure by (Perry & Chilton, 1973);

$$\Delta C_{Pg} = 4.184 \times 10^3 (T_R/1.686)^{-3.72} p_R^{0.9155}/M.W. \quad (9)$$

where ΔC_{Pg} = correction added to C_{Pg} to account for different pressure ($J/kg\ ^oK$)
T_R = reduced temperature (^oK)
= T/T_C
P_R = reduced pressure (N/m^2)
= P/P_C

The ratio of heat capacity at constant pressure to heat capacity at constant volume (C_{vg}) is given by (Perry & Chilton, 1973);

$$K = C_{Pg}/(C_{Pg}-[8.314\times10^{3}/M.W.]) \quad (10)$$

2.5.2 Liquid State

2.5.2.1 Liquid Density

Bhirud's method is used to calculate the liquid density (Lyman et al, 1982);

$$\rho_L = 10^{3}M.W.P_C/RT\ e^{(a+wb)} \quad (11)$$

and,

$$a = 1.396444-24.07T_R+102.615T_R^2- \quad (12)$$
$$255.719T_R^3+355.806T_R^4-$$
$$256.671T_R^5+75.1088T_R^6$$

$$b = 13.4412-135.7437T_R+533.380T_R^2- \quad (13)$$
$$1091.453T_R^3+1231.43T_R^4$$
$$-728.227T_R^5+176.737T_R^6$$

$$w = \frac{3}{7}(T_{BR}/[1-T_{BR}])\ (\log(P_C/1.01\times10^{5})-1)$$

where ρ_L = liquid density (kg/m^3)
a,b = constants
w = accentric factor
T_{BR} = reduced boiling point
= T_B/T_R
T_B = boiling point (^{o}K)

2.5.2.2 Liquid Heat Capacity

The heat capacity at constant pressure is calculated from the gas heat capacity at constant pressure by (Perry & Chilton, 1973);

$$C_{Pl} = C_{Pg} + (4.686 \times 10^4 / M.W.) \quad (14)$$

where C_{Pl} = liquid heat capacity at constant pressure (J/kg^oK)

2.5.2.3 Heat of Vaporization

The Reidel equation (Lyman et al, 1982) is used to estimate the heat of vaporization at the boiling point;

$$\Delta H_{VB} = \frac{4.184 \times 10^3 T_B (5 \log [P_C/1.01 \times 10^5] - 2.17)}{M.W. (0.930 - T_{BR})} \quad (15)$$

where ΔH_{VB} = heat of vaporization at the normal boiling point (J/kg)

This value is corrected for temperatures other than the normal boiling point using an adaption of the Thiesen correlation (Lyman et al, 1982);

$$\Delta H_V = \Delta H_{VB} ([1-T_R]/[1-T_{BR}])^{0.38} \quad (16)$$

2.5.2.4 Surface Tension

The liquid surface tension at the boiling point (it's only use in the model) is calculated using Walden's rule (Perry & Chilton, 1973);

$$\sigma = 6.56 \times 10^7 \Delta H_{VB} \rho_L$$

where σ = surface tension (N/m)

2.5.2.5 Kinematic Viscosity Ratio

The ratio of liquid to gas kinematic viscosity is determined by dividing Arrhenuis's relation for liquid viscosity by Arnold's correlation for gas viscosity (both converted from dynamic to kinematic terms) to yield;

$$\nu_L / \nu_V = 37 M.W.^{1/6} \rho_V (T+1.47T_B) / \rho_L^{7/6} T^{3/2} \qquad (17)$$

where ν_L/ν_V = ratio of liquid to gas kinematic viscosity

2.5.2.6 Vapour Pressure

The vapour pressure of the liquid is calculated using Riedel's analytical correlation (Perry & Chilton, 1973);

$$P_V = P_C / 10^{(0.118B - 7\log T_R + [\alpha_C - 7][0.0364B - \log T_R])}$$

and

$$B = (36/T_R) - 35 - T_R^6 + 42 \ln T_R$$

$$\alpha_C = 0.9076(1 + [T_{BR} \ln[P_C / 1.01 \times 10^5]] / [1 - T_{BR}])$$

2.6 GAS FLOW THROUGH RUPTURE

If the contents of the tank are gaseous (or only vapour is present) at elevated pressure the outflow rate is calculated as follows;

* first, the initial tank pressure is determined using the equation of state (equation 1) and:

  $\underline{V} = V_T M.W./CMASS \qquad (18)$

  where CMASS = mass of chemical in tank (kg)

* next, a series of calculations are performed to determine whether or not the flow is sonic or subsonic:

$$\beta = D_R/D_T \qquad (19)$$

where D_R = diameter of rupture (m)
= $2r_r$, for circular holes
= $(L_R W_R)^{1/2}$, for rectangular holes

D_T = diameter of tank
= 2r for cylindrical or spherical tanks
= $(LWh)^{1/3}$ for rectangular tanks

if $\beta \leq 0.2$

$$r_c = (2/[k+1])^{K/(K-1)} \qquad (20)$$

where r_c = critical pressure ratio for sonic flow

if $\beta > 0.2$

$$r_c^{(1-k)/k} + (k-1)\beta^4 r_c^{(2/k)}/2 = (k+1)/2 \qquad (21)$$

if $r_c \geq P_{atm}/P_{tank}$ sonic flow exists
if $r_c < P_{atm}/P_{tank}$ sub-sonic flow exists

where P_{atm} = atmospheric pressure (N/m^2)
P_{tank} = pressure in tank (N/m^2)

* The mass flow rate through the rupture is then determined by the appropriate sonic or sub-sonic flow equation.

2.6.1 Sonic Flow

$$\dot{m} = C_D A_R (K(P_T \rho_V)(2/[k+1])^{(k+1)/(k-1)})^{1/2} \qquad (22)$$

where C_D = discharge coefficient
= 0.61

A_R = area of rupture (m^2)
= r^2 for circular hole
= $L_R W_R$ for rectangular hole

$\dot{m}$ = mass flow through rupture (kg/s)

If the flow is initially sonic, the model calculates the mass flow for twenty uniform iterations from the initial tank pressure to the pressure at which subsonic flow commences.

2.6.2 Subsonic Flow

Assuming isentropic flow:

$$\dot{m} = C_D A_R Y (2(P_{tank}-P_{atm})\rho_V)^{1/2}/(1-\beta^4)^{1/2} \quad (23)$$

and

$$Y = 1-([1-r]/K)(0.41+0.35\beta^4) \quad (24)$$

where Y = expansion coefficient

r = pressure ratio

$= P_{atm}/P_{tank}$

The model then calculates the mass flow for twenty uniform iterations from the initial tank pressure (or from the pressure at which the flow becomes subsonic - see above) to atmospheric pressure.

No heat transfer calculations are required for either the sonic or subsonic gas flow model since the gas cools only as it expands isentropically through the rupture.

2.7 LIQUID FLOW THROUGH RUPTURE

For the case of a liquid whose vapour pressure is less than atmospheric pressure (i.e., its boiling point is above the ambient temperature) the flow through the rupture is incompressible and can be calculated from (Dodge et al, 1980).

$$\dot{m} = C_D A_R (2(P_{hole}-P_{atm})\rho_L)^{1/2}/(1-\beta^4)^{1/2} \quad (25)$$

and

$$P_{hole} = (h_L-h_R+D_R/2)\rho_L g + P_v \quad (26)$$

where P_{hole} = pressure in liquid at rupture centreline (N/m^2)

g = acceleration of gravity ($9.81\ m/s^2$)

The model calculates the liquid outlfow for increments of 5 cm drops in liquid level until either the pressure at the hole drops close to atmospheric pressure and air is ingested into the tank or the liquid level reaches the top of the hole. Once the latter occurs P_v is set at atmospheric pressure and the calculations continue in 5 cm increments until the bottom of the hole is reached, at which time the flow stops.

2.7.1 Air Ingestion

It is well known that once the pressure difference across the rupture approaches zero, air will be ingested into the tank and an equivalent volume of chemical flow out. This is accounted for in the model by using a variation of the approach proposed by Dodge et al, 1980. Once $P_{hole} \leq 1.01\ P_{atm}$, air ingestion begins at a volumetric rate equal to the liquid outflow which is equal to the mass flow from equation 25 with P_{hole} set at $1.01\ P_{atm}$. This continues in 5 cm increments of liquid level until the height of the liquid equals the height of the top of the hole. At this point P_v is set equal to P_{atm} and the model reverts to equations 25 and 26. This continues in 5 cm increments until the liquid level reaches the bottom of the hole and flow stops.

2.7.2 Evaporation Losses

Once the liquid level in the tank begins to drop the pressure in the vapour space falls. If this continues to a point where the pressure drops below the vapour pressure of the chemical evaporation of the liquid in the tank will begin. This is accounted for by (Dodge et al, 1980):

$$\dot{m}_e = \dot{m}_{esat'd} - (1.9(\dot{m}_{esat'd})^{5/4}/(\rho_L A_{SC}(RT)^{1/2})^{1/4}) \quad (27)$$

and

$$\dot{m}_{esat'd} = \rho_v \dot{m}/(\rho_L - \rho_v) \quad (28)$$

where $\dot{m}_e$ = mass evapration rate of liquid into vapour space (kg/s)

$\dot{m}_{esat'd}$ = theoretical equilibrium evaporation rate (kg/s) to fill vapour space as liquid level falls

The time required to discharge 5 cm of the liquid is then reduced by an amount proportional to the evaporation rate.

The evaporation process sets up a heat flow into the tank. This is discussed in the next section dealing with two-phase flow.

2.8 TWO-PHASE FLOW THROUGH RUPTURE

For liquids whose vapour pressure is greater than atmospheric pressure two situations can result in two-phase flow through the rupture. The first of these is flow through a hole below the liquid level at a rate sufficient to cause boiling of the liquid as the vapour space pressure decreases. The second is boiling and subsequent overflow caused by rapid depressurization of the vapour space from a hole above the liquid level. Both situations are extremely complex since heat tranfer, mass transfer and two-phase flow are occurring simultaneously.

2.8.1 Void Fraction

The most important factor in the two-phase flow model is the volumetric void fraction of vapour in the liquid (or its mass equivalent; quality). The void fraction, or "holdup", in a flashing liquid (due to depressurization) is calculated using Viecenz's experimental correlation (Mayinger, 1981):

$$\varepsilon = 0.73(U_{og}^2/g(\sigma/g(\rho_L-\rho_v))^{1/2})^{0.376}((\sigma/g(\rho_L-\rho_v))^{1/2}/D_{tank})^{0.176}(\rho_L/(\rho_L-\rho_v))^{0.585}$$

$$(\mu_L/\mu_v)^{0.256} \qquad (29)$$

in which

$$U_{og} = \dot{m}_e/\rho_v A_{sc} \qquad (30)$$

where ε = void fraction

U_{og} = superficial vapour velocity (m/s)

The stagnation quality is related to void fraction through:

$$X_o = \rho_v/(\rho_v+((1/\varepsilon)-1)+\rho_L) \qquad (31)$$

where X_o = stagnation quality or the mass fraction of vapour in the fluid

The presence of vapour bubbles in the tank creates an expansion in the fluid volume necessitating a redefinition of liquid height; one, the actual fluid level in the tank including vapour bubbles (h_L) and another an equivalent height of liquid if no bubbles were present (h_{LE}) which is used for pressure calculations. The fluid volumes which, in combination with tank geometry calculations, are used to determine h_L and h_{LE} are related by:

$$V_L = V_{LE}/(1-\varepsilon) \qquad (32)$$

2.8.2 Hole Below Liquid Level

2.8.2.1 Two-Phase Subsonic Flow

If the void fraction is greater than 0.01 the flow is considered two-phase and choking can occur (sonic flow). The critical pressure ratio is determined from (Henry, 1981)

$$r_c = e^{(-0.4353X_o-0.1625)} \qquad (33)$$

If $r_c > P_{atm}/P_{hole}$ the flow is subsonic. The mass flowrate is calculated by (Delhaye, 1981):

$$\dot{m} = C_D A_R Y(2(P_{hole}-P_{atm})/(X_o^{1.5}((1/\rho_v)-(1/\rho_L))+(1/\rho_L))^{1/2}/(1-\beta^4)^{1/2} \qquad (34)$$

In which Y, the expansion coefficient of the vapour is calculated as in the gas model (equation 24). Note that if X_o is 0, equation 34 becomes equation 25 with Y=1 for one phase incompressible flow. If X_o=1, equation 34 becomes equation 23 for one phase compressible flow.

2.8.2.2 Two-Phase Sonic Flow

If $r_c \leq P_{atm}/P_{hole}$ then the flow is sonic. The mass flowrate is given by (Henry, 1981):

$$\dot{m} = \frac{C_D A_R Y}{(1-\beta^4)^{1/2}}\left(2\rho_L P_{hole}(1-\varepsilon)\frac{(((1-\varepsilon)/\varepsilon)(1-r_c)+((k/(k-1))(1-r_c^{((k-1)/k)}))}{(1-X_o)\varepsilon(((1-\varepsilon)/\varepsilon)+r_c^{(-1/k)})^2}\right)^{1/2} \qquad (35)$$

As X_o and ε approach 1 equation 35 approaches equation 22 for one phase compressible critical flow.

2.8.3 Hole in Vapour Space

In the event of a hole in the vapour space the model starts by using the gas model (Section 2.6) for either sonic (equation 22) or subsonic (equation 23) flowrate.

As the pressure in the vapour space decreases, the liquid boils (equations 27 and 28), a fraction of vapour is held up in the liquid (equation 29 and 30) and the fluid expands (equation 32).

If the height of the flashing fluid reaches the rupture, the model calculates the outflow rate on the basis of either sonic (equation 35) or subsonic (equation 34) flow. At this point the rate of pressure loss due to vapour outflow is reduced by liquid flowing from the rupture, the vapour space pressure increases by vapour generation from the flashing liquid, the void fraction decreases, the fluid volume decreases and the liquid level drops below the rupture. The model then reverts to the gas flow equations and the process is repeated. This continues until the flashing liquid level no longer reaches the rupture, either because of fluid losses or evaporative cooling (combined with heat transfer - see below) at which point the driving force for the outflow is the vapour pressure of the chemical. Once the temperature of the liquid reaches its boiling point (ie the vapour pressure equals atmospheric pressure) the mass loss rate is equal to the evaporation rate as determined by heat transfer.

All the two-phase flow models use 5 cm increments in liquid level for determining flowrates.

2.9 HEAT TRANSFER

The key heat transfer process involved in the release of liquid chemicals from a rupture is cooling of the bulk liquid through evaporation (heat of vaporization and heat capacity of the chemical) combined with warming of the liquid by heat transferred from the environment through the tank walls. The balance of these two heat flows defines the temperature of the liquid and vapour (and thus their physical, chemical and thermodynamic properties) and the final rate at which low boiling liquids are released through ruptures in the vapour space.

The equation for determining the temperaure of the tank contents is:

$$T_{i+1} = T_i - ((\dot{m}_e \Delta H_v \Delta t_i) - (U_o A_{SA} \Delta t_i (T_{air} - T_i))) / \gamma_L V_{Li} C_{Pl} \qquad (36)$$

where T_i, T_{i+1} = temperature of liquid in tank before and after each iteration (^oK)

Δt_i = calculated time of outflow for each iteration (s)

U_o = overall heat transfer coefficient ($J/sm^2{}^oK$)

T_{air} = air temperature (^oK)

The overall heat transfer coefficient is determined as shown below.

2.9.1 Overall Heat Transfer Coefficient

$$U_o = 1/((1/h_i)+(x_w/k_w)+(x_I/k_I)+(1/h_o)) \quad (37)$$

where h_i, h_o = inside and outside heat transfer coefficeints ($J/m^2 s^oK$)

x_w, x_i = wall and insulation thickness (m) x_w is input or set at 0.01m; x_I is arbritarily set at either 0 or 0.1 m

K_w, K_i = wall and insulation thermal conductivities (J/ms^oK) K_w = 16.45 J/ms^oK (steel); K_i = 2.74×10^{-3} J/ms^oK (average for foam)

2.9.2 Outside Heat Transfer Coefficient

The outside heat transfer coefficient is calculated by (Perry & Chilton, 1973):

$$h_o = 0.017B(6.67 \times 10^4 Lv)^n/L \quad (38)$$

where v = wind speed (m/s)

L = tank dimension (m) - see below

B,n = constants defined by tank shape as shown in Table 4

TABLE 4

OUTSIDE HEAT TRANSFER COEFFICIENT CONSTANTS

TANK SHAPE	PARAMETER IN EQUATION 38		
	L	B	n
cylindrical	diameter	0.0266	0.805
spherical	diameter	0.6	0.5
rectangular	shortest dimension	0.104	0.675

2.9.3 Inside Heat Transfer Coefficient

The inside heat transfer coefficient is determined from one of two equations, depending on whether or not the liquid is boiling (Perry and Chilton, 1973);

for $T_i <$ boiling point

$$h_i = 69 \Delta T_{wall}^{1/4} / h_L^{1/4} \qquad (39)$$

where $\Delta T_{wall} = (T_{wall} - T_{air})$

T_{wall} = inside tank wall temperature (^{o}K)

Calculation of h_i requires an iterative procedure in which the first guess at T_{wall} is:

$$\Delta T_{wall_i} = (T_{air}-T_i)/2 \qquad (40)$$

h_i, h_o and U_o are then calculated and the next guess at T_{wall} is:

$$\Delta T_{wall_{i+1}} = U_o \ (T_{air}-T_i)/h_i \qquad (41)$$

The process continues until two successive iterations are within 2.5% of each other.

for $T_i \gg T_{boil}$

$$h_i = 3x10^{-6} P_C^{1.69} P_R^{0.35} (1-P_R)^{0.9} (1.8P_R^{0.17}+4P_R^{1.2}+10P_R^{10}) \qquad (42)$$

2.9.4 Insulation Losses

If an area of insulation around the rupture is destroyed the overall heat transfer coefficient is modified by summing the contributions to the total heat transfer of the insulated and uninsulated aeas:

$$U_o = U_o^I(1-(A_{ID}/A_{SA}))+U_o^{II}(A_{ID}/A_{SA}) \qquad (43)$$

where A_{ID} = area of insulation destroyed (m^2)
U_o^I = overall heat transfer coefficient including insulation ($J/m^2 s^oK$)
U_o^{II} = overall heat transfer coefficient excluding insulation ($J/m^2 s^oK$)

3.0 COMPUTER PROGRAM DESIGN

The general computer program structure, that integrates the equations presented in Section 2.0 is outlined in the following four flow charts (See Figures 1 to 4). A brief description of the workings of the model, based on these flowcharts follows. A complete program listing may be found in Appendix I.

3.1 MAINLINE PROGRAM STRUCTURE - "LEAKR"

The mainline program "LEAKR" controls the flow of the model by calling up the appropriate data imput and data manipulation routines. As is illustated in Figure 1, the chemical selection sub-routine "CHEM" is called which prompts the user to identify the chemical spilled and its initial temperature. The routine also supplies the mainline program with the 7 chemical characteristics required to calculate the chemical's physical and chemical properties as a function of temperature and pressure. Control is then passed to the environmental data imput sub-routine "ENVCON" which prompts the user for the air temperature, atmospheric pressure and wind speed at the spill site. The next routine called is the tank geometry input model "TANKG". The tank shape, wall thickness, insulation thickness, area of damaged insulation, and tank dimensions are all input at this stage in the program. Sub-routine "RUPTURE" is then called which prompts the user to select the rupture type (out of a possible 12) and enter the rupture size and location. The routine then selects the coefficient of discharge based on the puncture type selected. At this point the chemical properties needed in the discharge equations are initialized by calling sub-routine "INIT". "INIT" asks the user for the mass of chemical present in the tank and then calls upon either the "LEQNS" or "GEQNS" sub-routine to determine the initial chemical properties for the Liquid or Gas which is present. This routine then prints a listing of these initial chemical properties prior to carrying on. At this stage in "LEAKR" a check is made to determine which outflow model should be used to calculate the chemical discharge rate. If

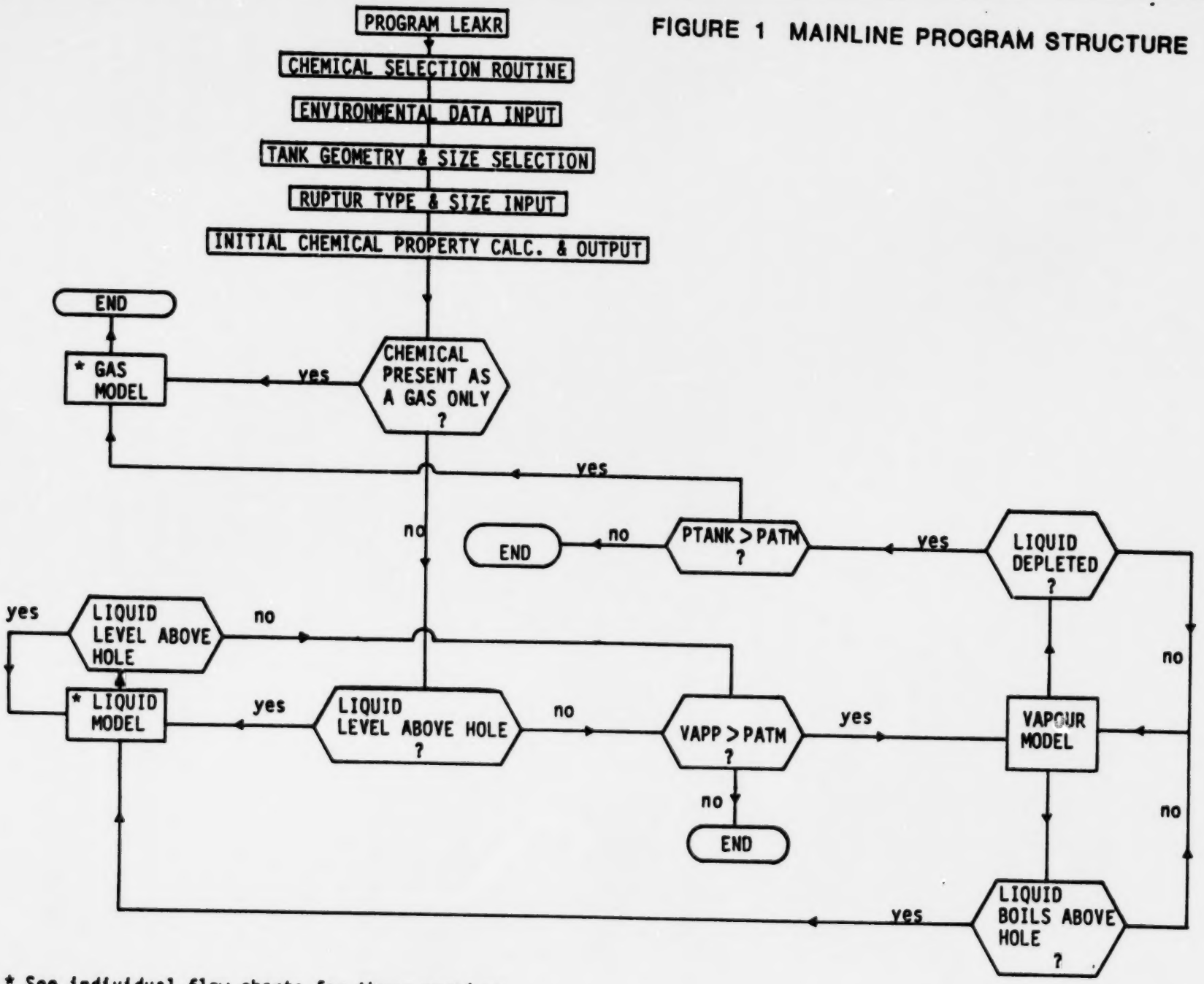
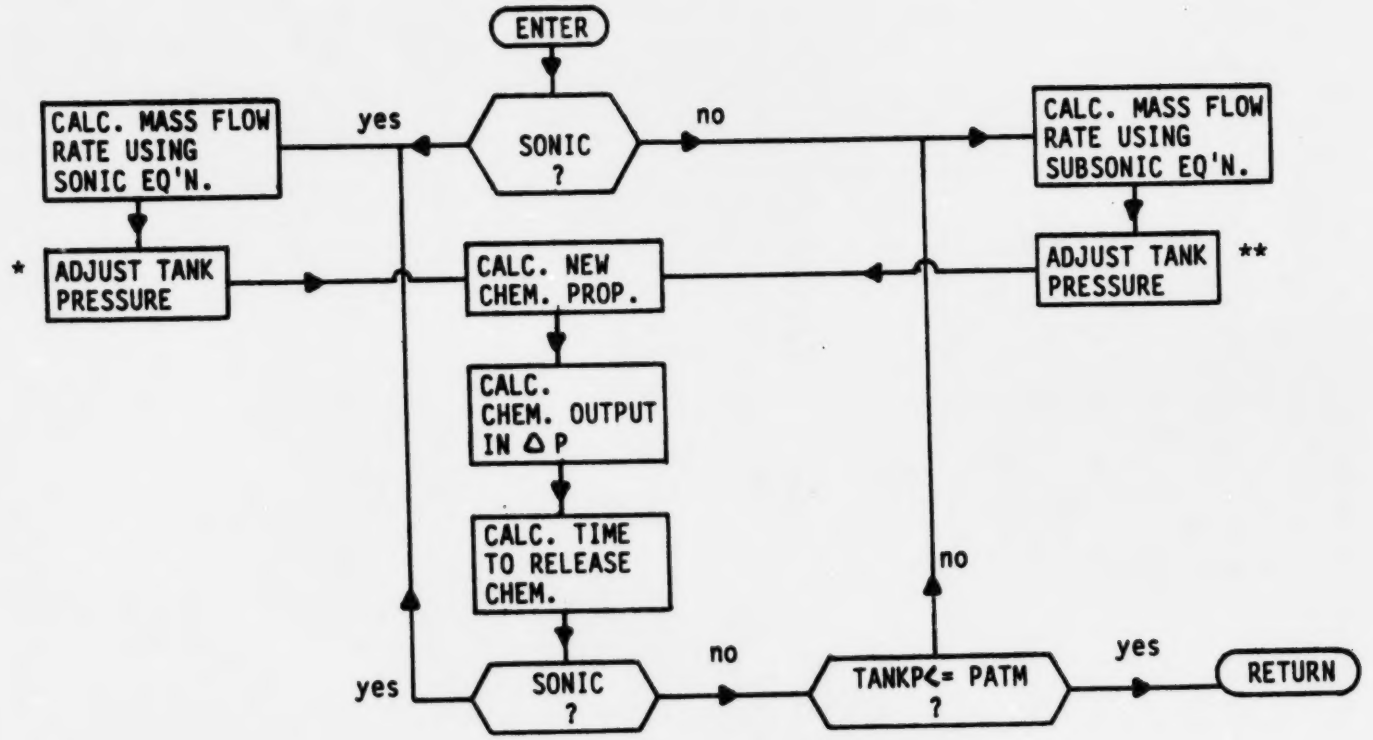


FIGURE 1 MAINLINE PROGRAM STRUCTURE

* See individual flow charts for these routines

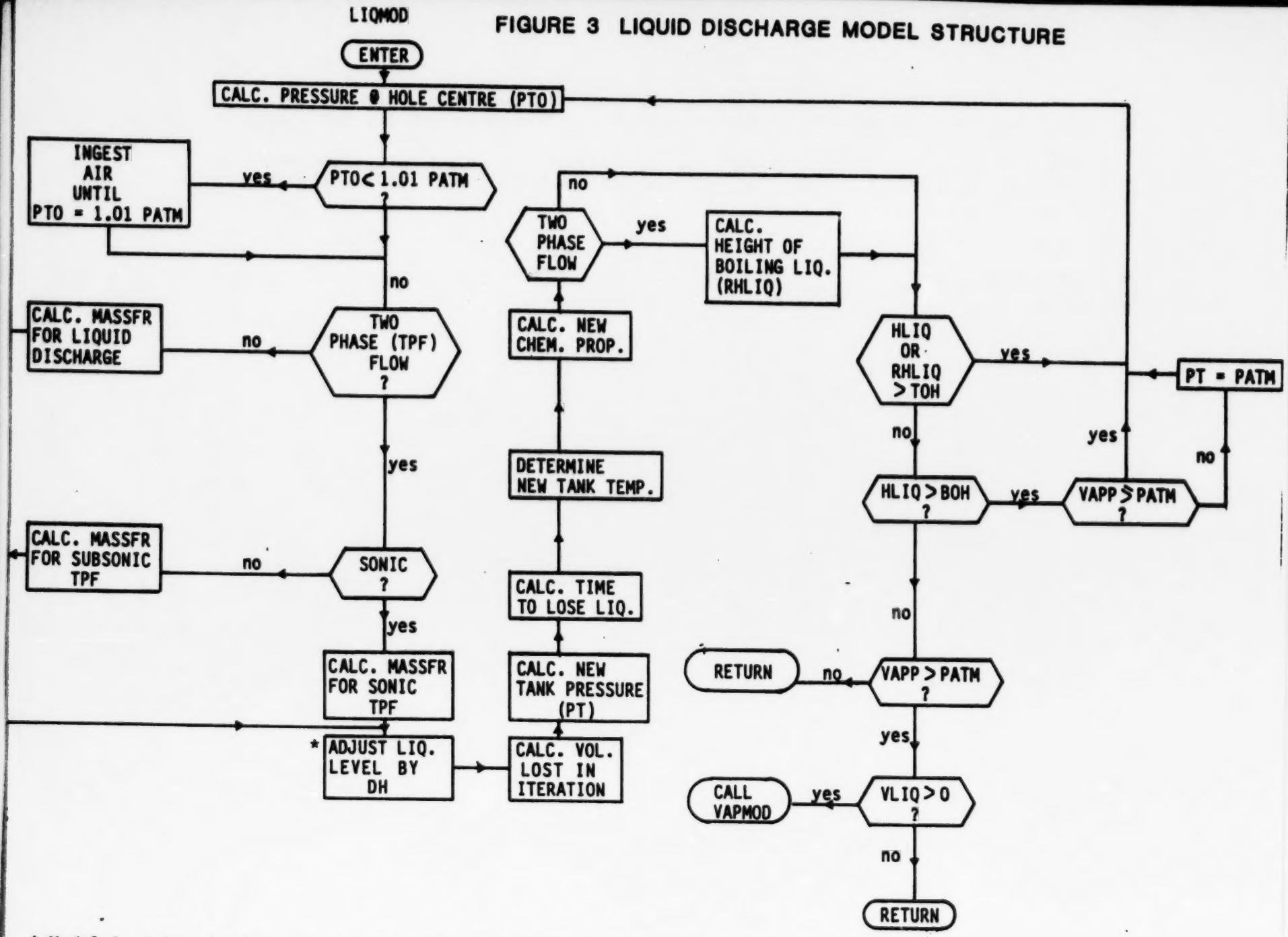
FIGURE 2 GAS DISCHARGE MODEL STRUCTURE



* If flow is sonic the pressure is dropped in 20 uniform iterations until sub-sonic flow is reached. Then control is transferred to the subsonic routine.

** Once subsonic flow is reached the pressure is dropped in 20 uniform iterations until the tank pressure = atmospheric pressure and discharge ceases.

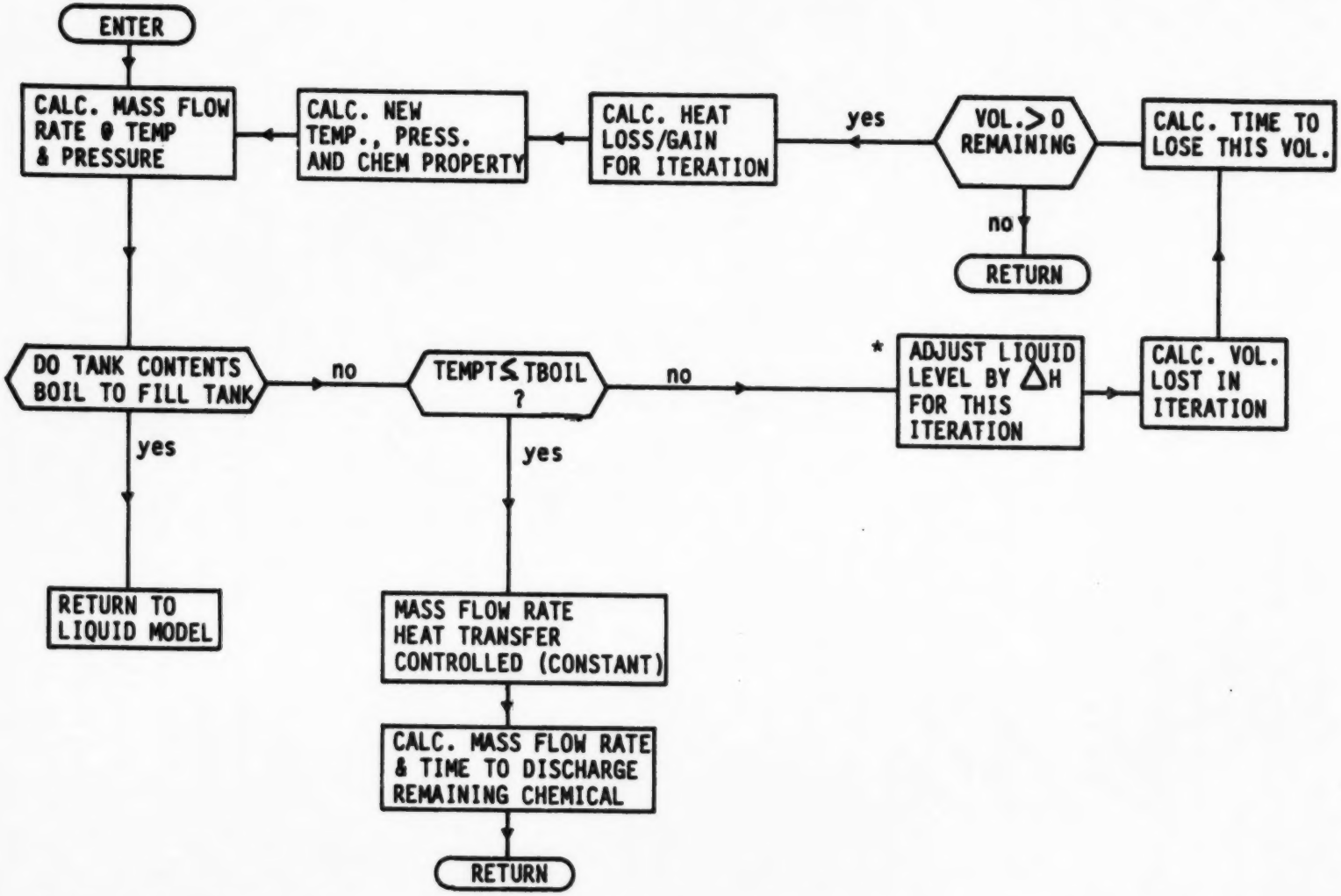
FIGURE 3 LIQUID DISCHARGE MODEL STRUCTURE



* Model is driven by iterations in liquid level and volumes lost with this change in level

FIGURE 4 VAPOUR DISCHARGE MODEL STRUCTURE

VAPMOD



* Note the model is driven by a constant change in liquid level for each iteration and the time it takes to evaporate and discharge this liquid volume

the chemical is present as a gas only control is transferred to the GAS model. All of the chemical is discharged via this model and the calculations are complete. Details of the GAS model are discussed in a following section. If the chemical is present as a liquid a check is made on the liquid level to see if it is above the "hole" bottom. If it is, transfer is passed to the liquid model, "LIQMOD", which handles the discharge of the chemical until the liquid level drops below the bottom of the hole. Details of this model can be found in Section 3.3. At this time a check is made to see if the chemicals vapour pressure is greater than atmospheric pressure. If it is not no more chemical will escape and the program terminates. This same check also occurs if the liquid level is initially below the bottom of the hole. If the vapour pressure (VAPP) is greater then atmospheric pressure control is passed to the vapour discharge model, "VAPMOD". Chemical escapes from the tank by boiling off from the liquid pool and escaping as vapour. If during this boiling the liquid level rises above the hole's bottom control is passed to the liquid model which discharges chemical until the liquid level again drops below the hole bottom. When all of the liquid is boiled off a check is made to see if the tank pressure is greater then atmospheric pressure. If it is, control is passed to the GAS model to discharge the remaining vapours in the tank. If the pressure is less than amospheric the program is terminated. The detailed workings of the GAS, LIQUID and VAPOUR models follow.

3.2 GAS DISCHARGE MODEL - "GASMOD"

When control is passed to the gas model an initial check is made to determine if the discharge is sonic or sub-sonic. The appropriate discharge equation is selected to determine the mass flow rate at the existing tank pressure. This mass flow rate is assumed to take place until the pressure drops a pre-determined amount. The new chemical properties are calculated at this new pressure. Knowing the gas density at the old and new pressure then allows the calculation of the amount of chemical lost during the pressure drop. The time to release this mass of chemical is then

calculated using the mass flow rate at the initial pressure and the total mass lost. Finally a check is made to determine if sonic or sub-sonic flow exists. If the flow is sonic the process is repeated until sub-sonic flow exists; if the flow is sub-sonic the process is repeated until the tank pressure falls below atmospheric and the routine ends. If the flow is initially sonic 20 iterations of the sonic discharge equation (in 20 uniform pressure drops) are completed to bring the discharge to a sub-sonic condition. Once the flow is sub-sonic 20 terations of the sub-sonic equation are carried out (again in 20 equal pressure drops) to discharge the remaining mass of chemical (atmospheric pressure is reached in the tank).

3.3 LIQUID DISCHARGE MODEL - "LIQMOD"

The first step in the liquid discharge model is the calculation of pressure at the puncture centre (tank pressure + head of liquid over hole). If the pressure is greater than 1.01 x atmospheric pressure liquid will flow out. If it is not air is ingested (@ Patm) until the pressure increases to allow the liquid to flow. At this point the program checks for a two-phase flow condition. If this does not exist the simple liquid discharge model is implemented to calculate the mass outflow rate. If two-phase flow exists a check is made to determine if it is sonic or sub-sonic and the routine branches to the appropriate mass flow rate equation to calculate this mass flow rate. After the calculation of the mass flow rate the liquid level is dropped by a uniform amount (0.05 metre was used in the model) and the volume of liquid the function lost by the drop in liquid level is calculated by determining the new liquid volume (using the function sub-routine "VOL") and subtracting from the old volume. The new tank pressure is then calculated by a simple ideal gas relationship. The time to lose this volume of liquid is then determined by dividing the total mass of liquid lost by the mass flow rate plus the evaporation rate. This then accounts for the fact that some of the liquid is simply lost to the vapour space and is not actually discharged from the tank. The new tank temperature is calculated by first reducing its

temperature due to evaporative heat loss (based on the evaporation rate) and then by calling the heat transfer routine "TEMP" to adjust the temperature of the tank due to heat loss/gain to the surrounding environment. The new chemical properties are then calculated using the sub-routine "LEQNS". If the flow is two-phase the height of the boiling liquid is calculated and then a check is made to see if the liquid is still above the top of the hole. If it is the process is started again with the calculation of the pressure at the rupture centre. If it is not above the top of the hole a check is made to see if it is above the bottom of the hole. If it is the vapour pressure is checked against the prevailing atmospheric pressure and the larger of the two is assigned to this tank pressure. If the liquid level drops below the hole the vapour pressure is again compared to atmospheric. If it is less than equal to atmospheric the program ends as no more chemicl will be discharged. If the vapour presure is greater than Patm and there is still liquid in the tank control is passed to the vapour model to discharge the remaining liquid. If there is no liquid left control is passed back to the main line routine where the remaining chemical will be discharged using the gas model, "GASMOD".

3.4 VAPOUR RELEASE MODEL - "VAPMOD"

Upon entering the "VAPMOD" routine the mass flow rate is calculated for the existing temperature and pressure conditions (the appropriate sonic or sub-sonic operations are used. If the liquid boils violently to fill the tank (or raise the liquid level above the bottom of the puncture) control is passed back to the liquid model after adjusting the tank temperature, due to the evaporative heat losses, and calculating the new chemical properties. If the liquid does not boil above the hole a check is made on the tank's temperature. If the temperature of the chemical is less than or equal to its boiling temperature the mass outflow is then controlled only by the heat transfer into the tank. The time to discharge the remaining chemical is then calculated in one step and the program ends. If the temperature of the chemical is above its boiling point

the routine continues. The liquid level is adjusted by DH (0.05 metres) and the volume of liquid lost is again determined by the function sub-routine "VOL". The time to lose the chemical is calculated by dividing the mass of liquid lost by the evaporation rate (which in turn is a function of the mass flow rate out of the puncture). The evaporation rate is used here because the only way the liquid level can drop is by evaporation. If there is liquid remaining in the tank the new tank temperature is calculated using the heat transfer routine and the evaporative heat losses. The new tank pressure is calculated and finally the chemical properties are re-evaluated. The routine is then repeated.

4.0 MODEL RESULTS

Unfortunately suitable field or laboratory data could not be found in the literature to allow validation of the model's output. The accuracy of the model is therefore unknown.

Nomographs similar to those presented in the TIPS manuals have been prepared for Ammonia, Chlorine, Benzene and Hydrogen Sulphide. These graphs are presented as Figures 5 to 11. It was not possible to run the model for Sulphuric Acid as several of the required constants were not available. Also included on each of these figures are the original TIPS leak rate predictions. The following can be said about the comparison of the two sets of results:

i) For benzene, the chemical with the lowest vapour pressure, the discharge from a hole in the bottom of a tank car predicted by the new model was slower then that from the original TIPS results for all rupture sizes. See Figure 5.

ii) For the remaining chemicals, all low boiling point liquids with high vapour pressures, the new model predicted a faster release of chemical for punctures in the tank bottom except for the smallest hole size (50 mm) where the results were very similar to those in the EnviroTIPS Manuals.

It should be noted that these differences in release rate predictions (for high vapour pressure chemicals and holes in the bottom of tank cars) are not really significant from a countermeasures or safety point of view, since the total release times predicted by the two methods lie between about 0.1 to 10 minutes.

iii) A major difference between the EnviroTIPS results and the new model's predictions arises when a comparison is made of the results for holes in the top of the tank car. Because of the heat transfer component in the new model its discharge predictions are much slower than the TIPS results. The flattening out of the curves for the new predictions is a result of the tank temperature dropping to the boiling point of the liquid at which time the heat transfer controls the evaporation process and therefore the chemical release rate.

FIGURE 5

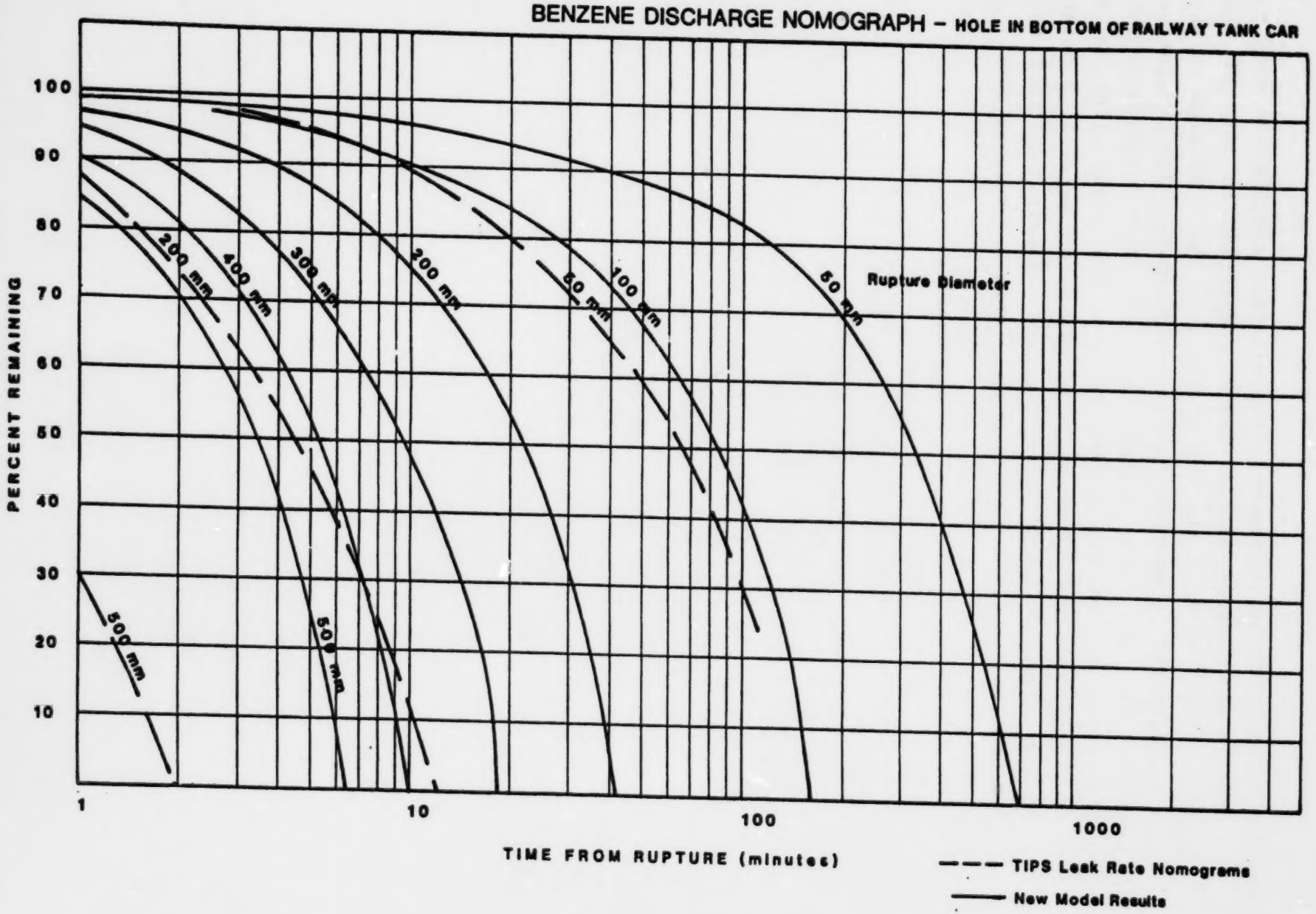

BENZENE DISCHARGE NOMOGRAPH – HOLE IN BOTTOM OF RAILWAY TANK CAR
PERCENT REMAINING
100
90
80
70
60
50
40
30
20
10
1
10
100
1000
TIME FROM RUPTURE (minutes)
Rupture Diameter
200 mm
400 mm
300 mm
200 mm
50 mm
100 mm
50 mm
500 mm
500 mm
TIPS Leak Rate Nomograms
New Model Results

FIGURE 6

CHLORINE DISCHARGE NOMOGRAPH – HOLE IN BOTTOM OF RAILWAY TANK CAR

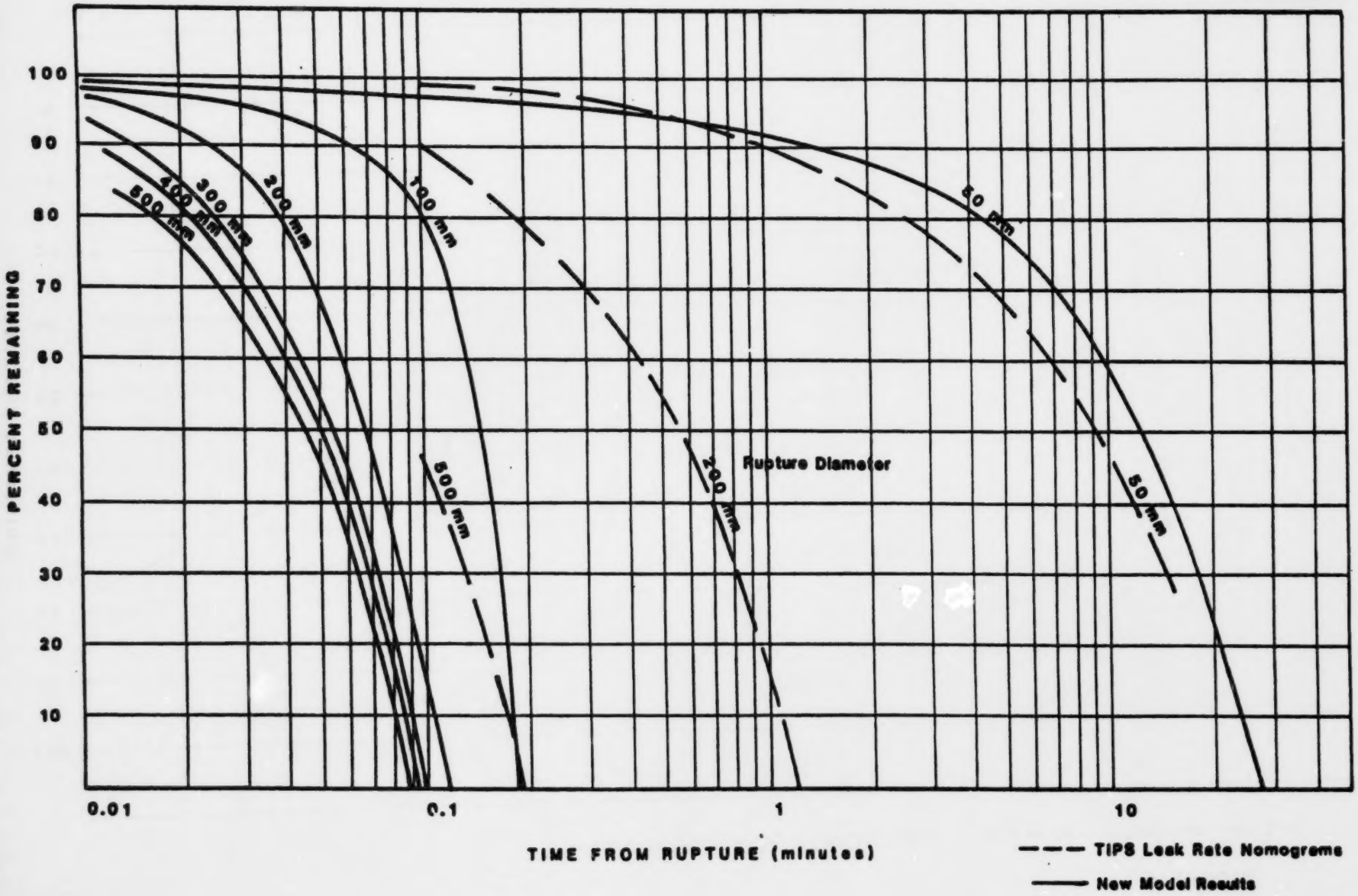


FIGURE 7

CHLORINE DISCHARGE NOMOGRAPH – HOLE IN TOP OF RAILWAY TANK CAR

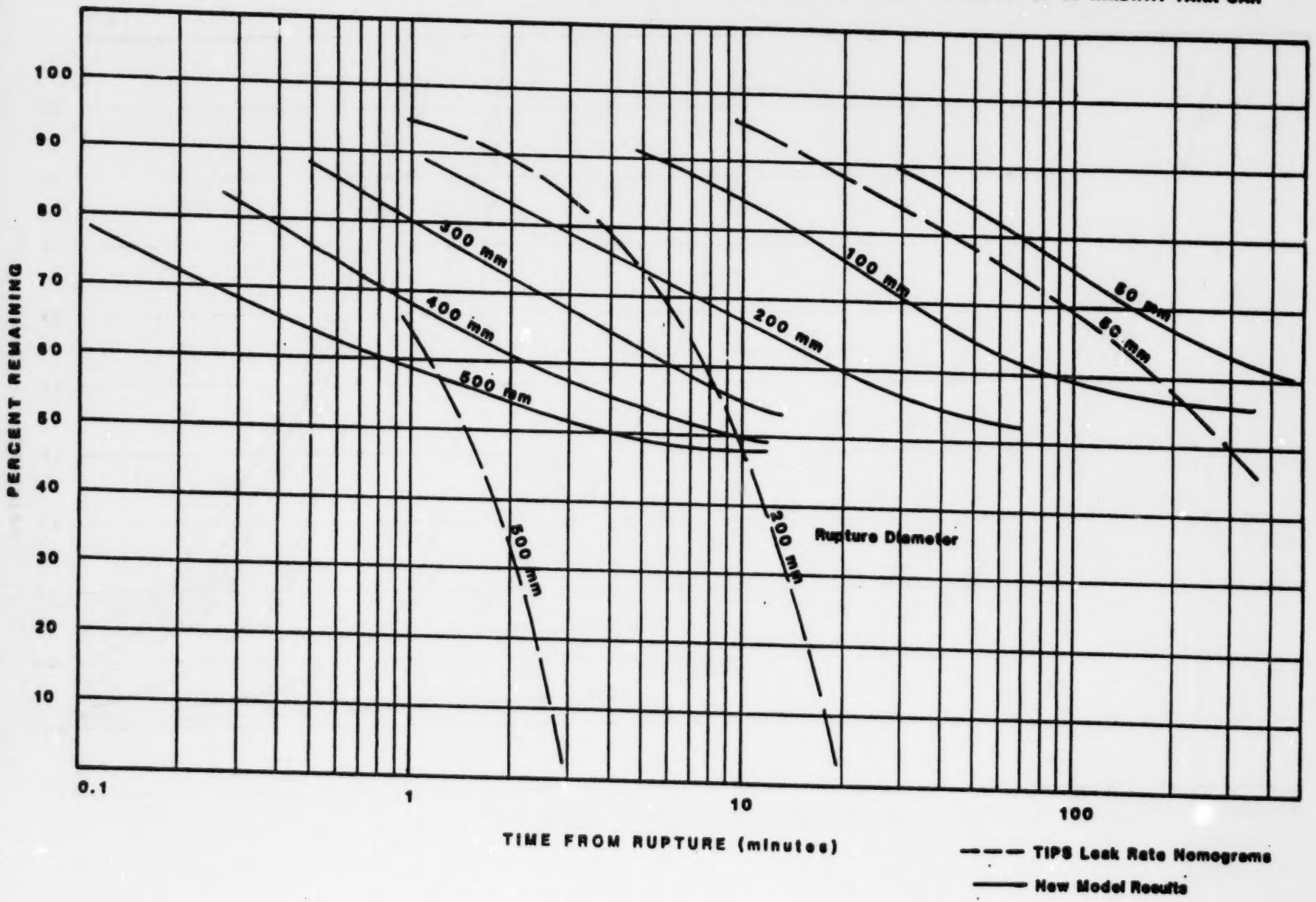


FIGURE 8

AMMONIA DISCHARGE NOMOGRAPH – HOLE IN BOTTOM OF RAILWAY TANK CAR

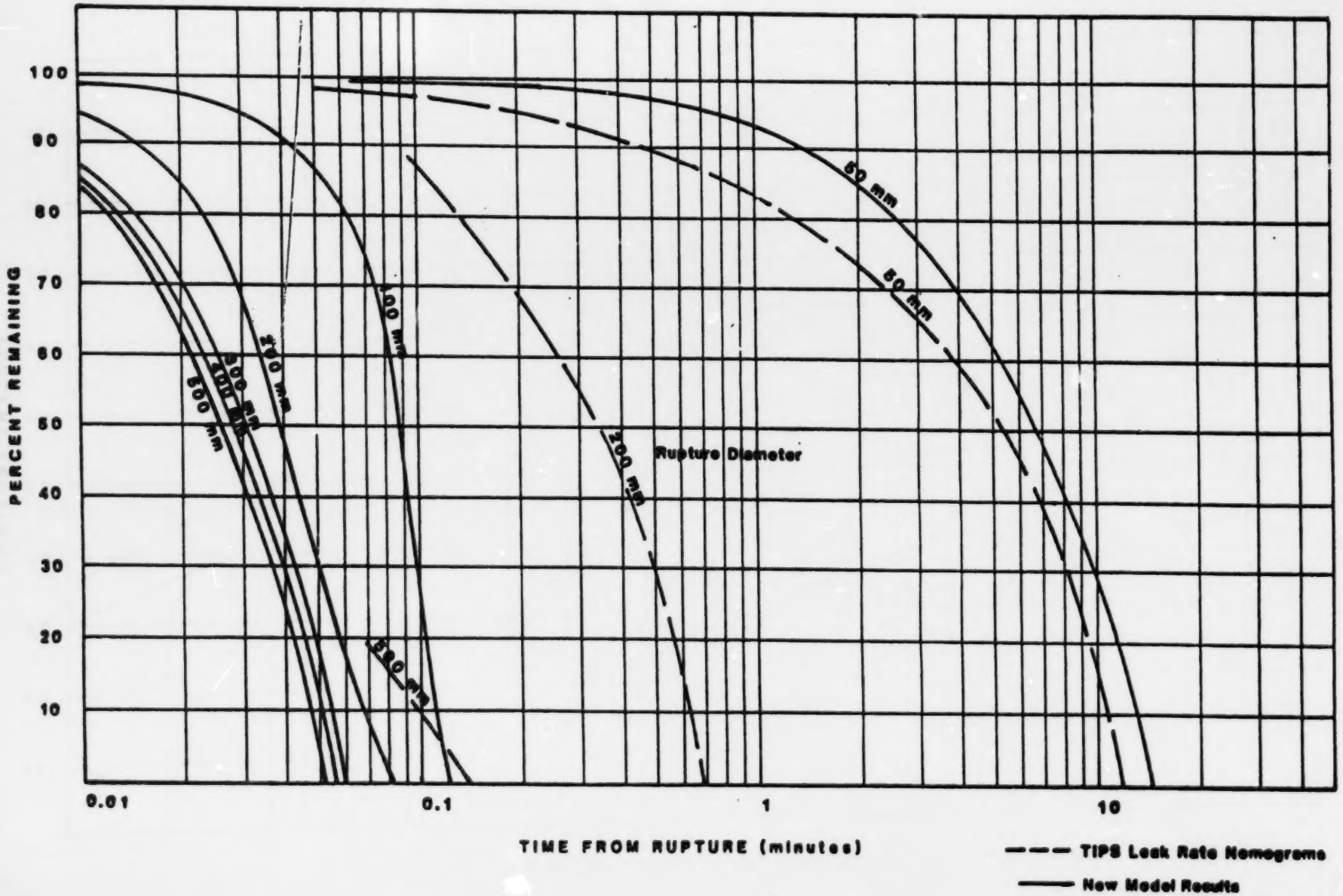


FIGURE 9

AMMONIA DISCHARGE NOMOGRAPH – HOLE IN TOP OF RAILWAY TANK CAR

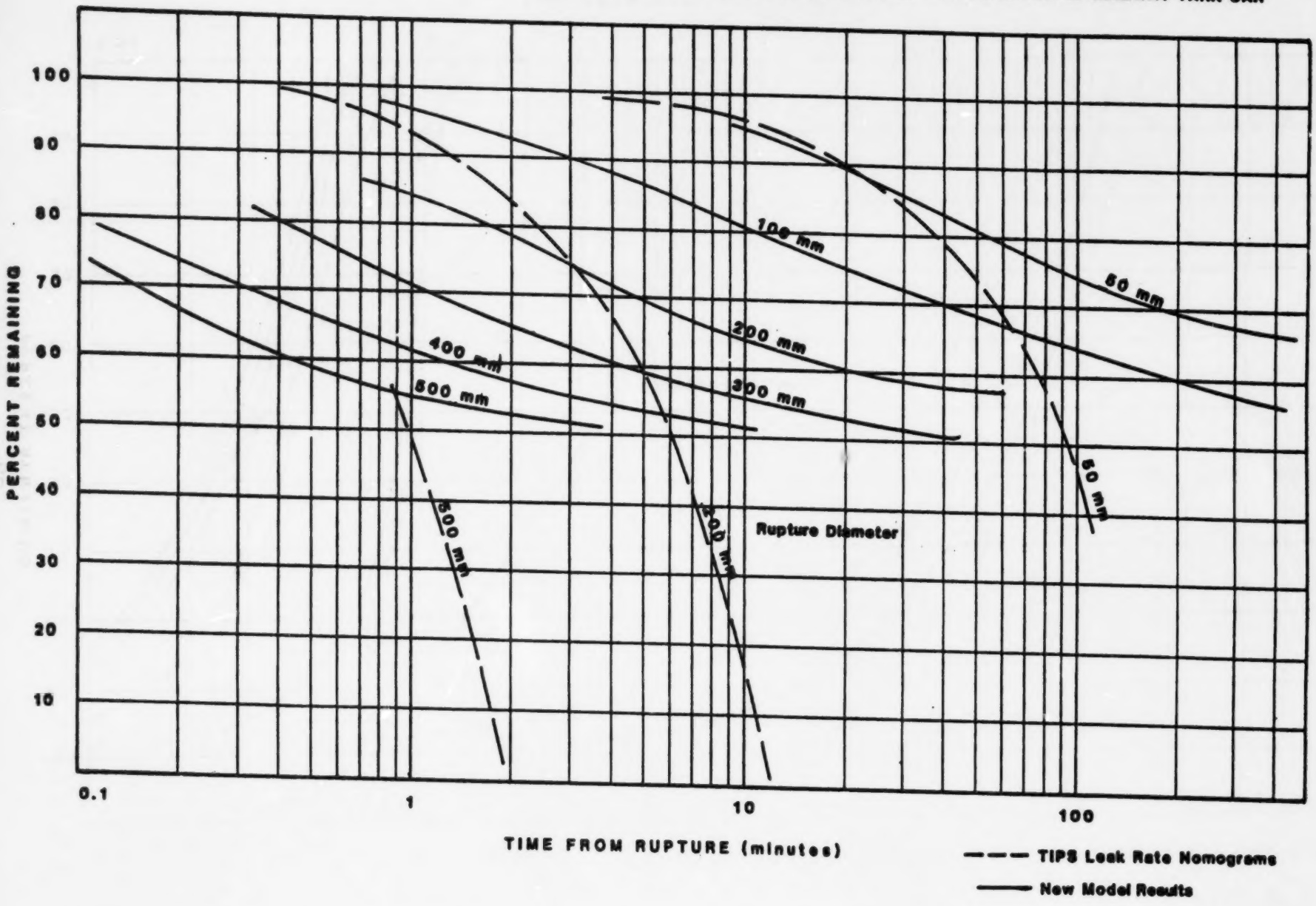


FIGURE 10

HYDROGEN SULPHIDE DISCHARGE NOMOGRAPH – HOLE IN BOTTOM OF RAILWAY TANK CAR

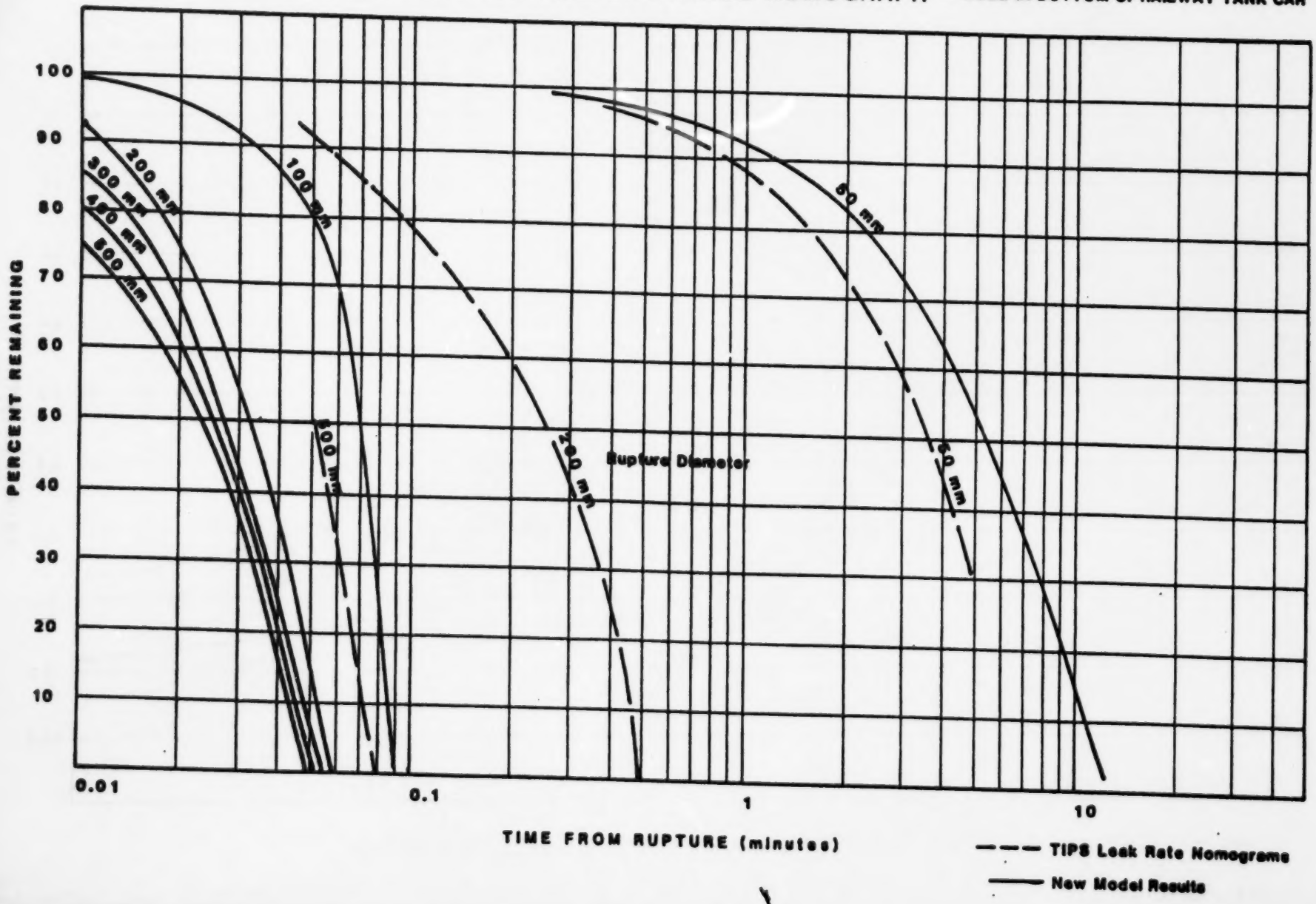
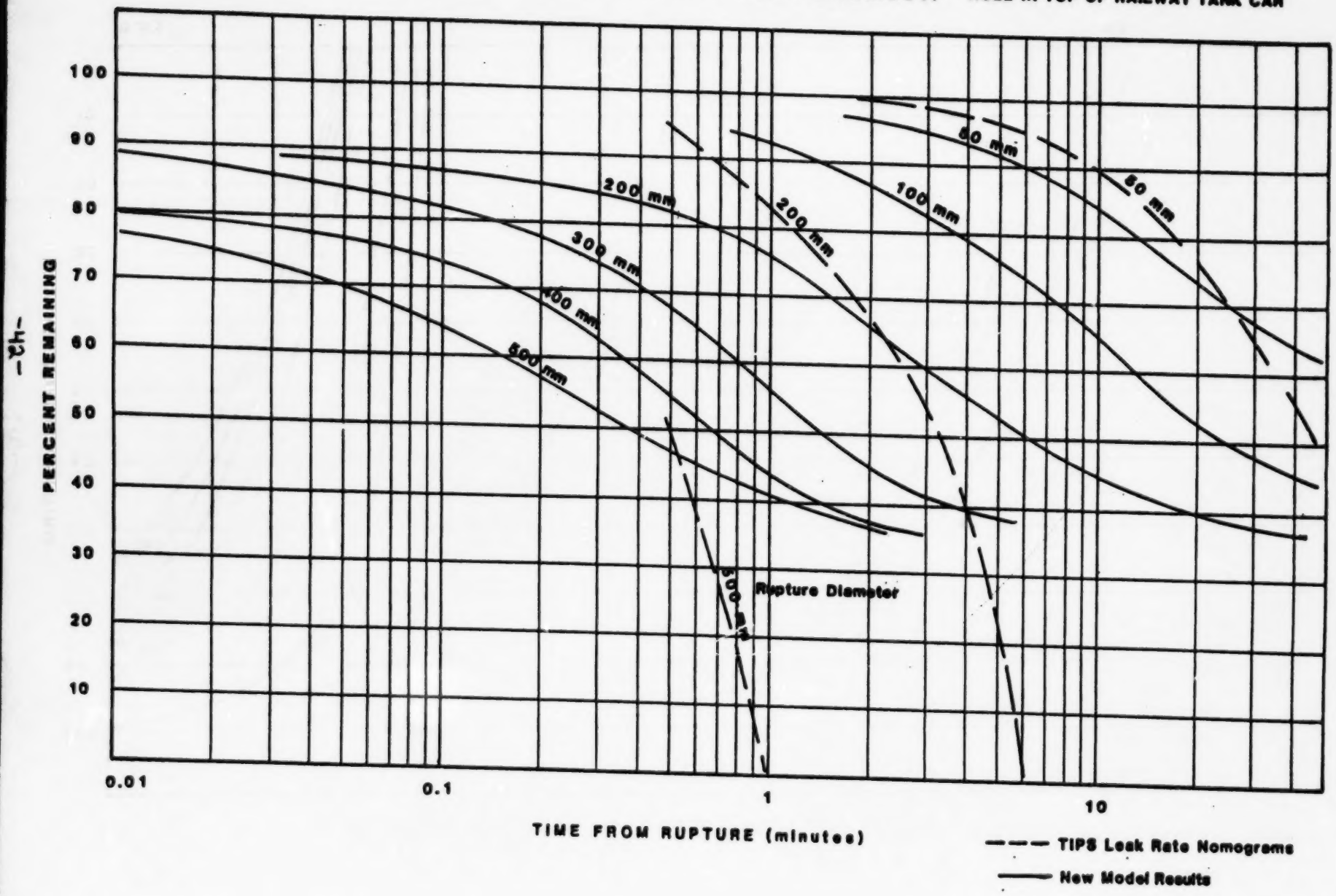


FIGURE 11

HYDROGEN SULPHIDE DISCHARGE NOMOGRAPH – HOLE IN TOP OF RAILWAY TANK CAR



5.0 CONCLUSIONS AND RECOMMENDATIONS

5.1 CONCLUSIONS

1) A simple-to-use computerized model to determine the rate and duration of leaks from chemical storge and transportation tanks has been developed.

2) The model is very flexible, capable of handling a wide range of tank and rupture sizes and shapes.

3) No knowledge of chemical properties (other than name and the amount in the tank) is required to operate the model.

4) Significant differences between the EnviroTIPS predictions and the computer model predictions exist for the cases of a puncture in the vapour space of tanks containing liquefied gases (chemicals with vapour pressures exceeding atmospheric at ambient temperaures).

5.2 RECOMMENDATIONS

1) Simple small and meso-scale tests should be carried out to validate the model.

2) The selection of chemicals stored in the program should be extended to include the most commonly spilled materials.

3) Once a generally accepted atmospheric dispersion model is available, the leak rate model should be configured to link with it.

4) Since it is virtually impossible to determine rupture size and shape at the scene of an accident a technique to determine this should be researched.

5) The model should be extended to permit the user to select the output desired (ie duration, maximum flowrate, chemical properties, etc).

6.0 REFERENCES

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APPENDIX I - COMPUTER PROGRAM LISTING

```
      PROGRAM LEAKR
      COMMON /CPROP/ TBOIL,TCRIT,PCRIT,RMW,A,B,C,IGAS,ICHEM
      COMMON /ENV/ TAIR,PATM,WINDS
      COMMON /TANK/ ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK,WALLT,
     +TINS,AINSD
      COMMON /RUPT/ IRUPT,HOLEH,RUPTA,CD,RUPTD,RUPTH,RUPTW,TOH,BOH
      COMMON /EQNS/ CMASS,DLIQ,VLIQ,HLIQ,PT,VAPD,VAPP,HCAPG,RK,HCAPL,DHV
     +,VLIQI
      COMMON /MOD/ CTIME,EE,BETA,I,IJ,UO,HTAREA,JCALL,K
      OPEN(1,FILE='LPT1:')
      CALL CHEM(TEMPTI)
      TEMPT=TEMPTI
      write(*,100)TEMPT
100   FORMAT(30X,F10.1,/,/)
      CALL ENVCON
      CALL TANKG
      CALL RUPTUR(IGAS)
      CALL INIT(TEMPT)
C
C** SELECT MASS OUTFLOW ROUTINE
C
      K=0
      I=9
      IJ=0
      CTIME=0.0
      JCALL=0
      ITPF=0
      PRAT=VAPP/PATM
      IF (IGAS.GT.0)GO TO 5
      IF(IRUPT.GT.4)DUM=RUPTH/2
      IF(IRUPT.LE.4)DUM=RUPTD/2
      IF(HOLEH-DUM.LT.HLIQ)CALL LIQMOD(TEMPT,ITPF)
      IF (JCALL.EQ.99) GO TO 6
      IF(HOLEH-DUM.GE.HLIQ) CALL VAPMOD(TEMPT)
      IF(JCALL .EQ. 99) GO TO 5
      CALL LIQMOD(TEMPT,ITPF)
5     IF(PT .LE. PATM) GO TO 6
      CALL GASMOD(TEMPT)
6     STOP
      END
      SUBROUTINE CHEM(TEMPTI)
      COMMON /CPROP/ TBOIL,TCRIT,PCRIT,RMW,A,B,C,IGAS,ICHEM
100   CONTINUE
      WRITE(*,1000)
1000  FORMAT('1',/,/,/,15X,'* *  CHEMICAL SELECTION MENU  * *',/,/)
      WRITE(*,1001)
1001  FORMAT(10X,
     +'AMMONIA          -  1',/,/,10X,
     +'BENZENE          -  2',/,/,10X,
     +'CHLORINE         -  3',/,/,10X,
     +'H2S              -  4',/,/,10X,
     +'SULPHURIC ACID   -  5',/,/,10X,
     +'ETHYLENE         -  6',1(/,))
      WRITE(*,1002)
1002  FORMAT(5X,'SELECT CHEMICAL BEING SPILLED  [# then RETURN] - ')
```

```
      READ(*,1003)ICHEM
1003  FORMAT(I2)
      WRITE(*,200)
200   FORMAT(5X,/,5X,'ENTER INITIAL TEMPERATURE OF TANK CONTENTS
     +[deg KELVIN : C+273 ]  - ')
      READ(*,201)DUMT
      TEMPTI=DUMT
201   FORMAT(F6.1)
      WRITE(*,1010)ICHEM,TEMPTI
1010  FORMAT('0',5X,'CHEMICAL SELECTED WAS # - ',I2,/,
     +5X,'INITIAL TANK TEMP INPUT WAS - ',F6.1,/,/,
     +5X,'IF DIFFERENT CHEMICAL WANTED ENTER 9 * otherwise * RETURN -')
      READ(*,1011)ICHK
1011  FORMAT(I2)
      IF (ICHK.GT.0)GO TO 100
C**
C**   GET APPROPRIATE CHEMICAL PROPERTIES
C**
      GO TO (31,32,33,34,35,36),ICHEM
C**   AMMONIA
31    TBOIL=239.6
      TCRIT=405.4
      PCRIT=113.0E05
      RMW=17.03
      A=6.086
      B=8.812E-03
      C=-1.506E-06
      IGAS=0
      GO TO 300
C**  BENZENE
32    TBOIL=353.1
      TCRIT=561.5
      PCRIT= 48.3E05
      RMW=78.11
      A=-0.409
      B=77.621E-03
      C=-26.429E-06
      IGAS=0
      GO TO 300
C**  CHLORINE
33    TBOIL=238.4
      TCRIT=417.0
      PCRIT= 77.1E05
      RMW=70.91
      A=7.576
      B=2.424E-03
      C=-.965E-06
      IGAS=0
      GO TO 300
C**  H2S
34    TBOIL=213.4
      TCRIT=373.4
      PCRIT= 90.1E05
      RMW=34.08
      A=6.662
```

```
            B=5.134E-03
            C=-.854E-06
            IGAS=0
            GO TO 300
C** SULPHURIC ACID
35          TBOIL=563.0
            TCRIT=99999
            PCRIT= 9999999
            RMW=116.09
            A=999999
            B=99999
            C=99999
            IGAS=0
C** ETHYLENE
36          TBOIL=169.1
            TCRIT=282.7
            PCRIT=5.117E06
            RMW=28.05
            A=2.83
            B=28.601E-03
            C=-8.7262E-06
            IGAS=1
300         RETURN
            END
            SUBROUTINE ENVCON
            COMMON /ENV/ TAIR,PATM,WINDS
100         CONTINUE
            WRITE(*,1000)
1000    FORMAT('1',9(/,),15X,'* * INPUT ENVIRONMENTAL CONDITIONS * *',/,/)
            WRITE(*,1001)
1001    FORMAT('0',10X,'ENTER AIR TEMPERATURE - deg KELVIN ( C+273).. - ')
            READ (*,1002) TAIR
1002        FORMAT (F8.1)
            WRITE(*,1003)
1003    FORMAT('0',10X,'ENTER ATMOSPHERIC PRESSURE (N/SQ M)..... - ')
            READ(*,1002)PATM
            WRITE(*,1004)
1004    FORMAT('0',10X,'ENTER WIND SPEED (M/SEC)..... - ')
C           READ(*,1002)WINDS
C** DATA CHECK
C
            WRITE(*,1006)TAIR,PATM,WINDS
1006        FORMAT('0',/,/,15X,
     +'AIR TEMP ..... - ',F8.1,/,15X,
     +'ATM. PRESSURE .... - ',F8.1,/,15X,
     +'WIND SPEED ..... - ',F8.1,/,15X,
            WRITE(*,1007)
1007        FORMAT(5X,'IF DATA ENTERED CORRECTLY - RETURN -',/,20X,
     +' OTHERWISE ENTER * 9 *  - ')
            READ (*,1008)ICHK
1008        FORMAT(I2)
            IF (ICHK.GT.0)GO TO 100
            RETURN
            END
```

```
      SUBROUTINE TANKG
      COMMON /TANK/ ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK,WALLT,
     +TINS,AINSD
100   CONTINUE
      WRITE(*,1000)
1000  FORMAT('1',/,/,/,/,/,20X,' * * TANK GEOMETRY SELECTION * * ',/,/)
      WRITE(*,1001)
1001  FORMAT(10X,
     +'RECTANGULAR ................. - 1',/,10X,
     +'CYLINDRICAL -horizontal .... - 2',/,10X,
     +'CYLINDRICAL -upright ....... - 3',/,10x,
     +'SPHERICAL  ................. - 4',5(/,))
      WRITE(*,1002)
1002  FORMAT(6X,'SELECT TANK SHAPE BY NUMBER then RETURN .............
     +...- ')
      READ(*,1003)ITANK
1003  FORMAT(I2)
      WRITE(*,999)
999   FORMAT('0',5X,'ENTER TANK WALL THICKNESS [METRES]',/,30X,
     +'(RETURN FOR DEFAULT VALUE) .......- ')
      READ(*,1008)WALLT
      IF (WALLT .EQ. 0.0) WALLT=.01
      WRITE(*,998)
998   FORMAT('0',5X,'ENTER INSULATION THICKNESS [METRES] ',/,30X,
     + '(0.0 IF NO INSULATION IS PRESENT)',/,30X,
     + '(0.1 IF THICKNESS UNKNOWN) .......- ')
      READ(*,1008)TINS
      WRITE(*,997)
997   FORMAT('0',5X,'ENTER AREA OF INSULATION LOST DUE TO RUPTURE',/,30X
     +,'[SQUARE METRES] .................- ')
      READ(*,1008)AINSD
      WRITE(*,1004)ITANK,WALLT,TINS,AINSD
1004  FORMAT(5X,
     +'TANK TYPE SELECTED WAS ...... -',6X,I2,/,5X,
     +'TANK WALL THICKNESS ......... -',F8.2,/,5X,
     +'THICKNESS OF INSULATION ..... -',F8.2,/,5X,
     +'AREA OF INSULATION DAMAGED .. -',F8.2,/,5X,/,/)
      WRITE(*,1005)
1005  FORMAT(5X,'IF SELECTION O.K. just RETURN otherwise ENTER  * 9 *
     +.....- ')
      READ(*,1003)ICHK
      IF(ICHK.GT.0)GO TO 100
200   CONTINUE
C
C**   ENTER TANK DIMENSIONS
C
      GO TO (21,22,22,23),ITANK
C*    RECTANGULAR
21    WRITE(*,1007)
1007  FORMAT('0',/,/,15X,'** RECTANGULAR TANK DIMENSIONS **',/,/,/,11X,
     +'ENTER HORIZONTAL LENGTH [METRES] ..........- ')
      READ(*,1008)TANKL
1008  FORMAT(F8.2)
      WRITE(*,1009)
1009  FORMAT('0',10X,'ENTER VERTICAL HEIGHT OF TANK [METRES] ....- ')
```

```
      READ (*,1008)TANKH
      WRITE(*,1010)
1010  FORMAT('0',10X,'ENTER WIDTH OF TANK [METRES] ..............- ')
      READ(*,1008)TANKW
      WRITE(*,1011) TANKL,TANKH,TANKW
1011  FORMAT('0',4X,
     +'TANK LENGTH .... -',F8.2,/,5X,
     +'TANK HEIGHT .... -',F8.2,/,5X,
     +'TANK WIDTH ..... -',F8.2,/,/)
      WRITE(*,1012)
1012  FORMAT(5X,'IF DIMENSIONS O.K. RETURN otherwise ENTER 9 - ')
      READ(*,1003)ICHK
      IF (ICHK.GT.0)GO TO 200
      VTANK=TANKL*TANKH*TANKW
      TANKP=0.0
      TANKD=0.0
      RETURN
C
C**   CYLINDRICAL TANK
22    WRITE(*,1014)
1014  FORMAT('0',/,/,15X,'** CYLINDRICAL TANK DIMENSIONS **',/,/,/,11X,
     +'ENTER DIAMETER OF CYLINDER [METRES] ......- ')
      READ(*,1008)TANKD
      WRITE(*,1015)
1015  FORMAT('0',10X,'ENTER LENGTH OF CYLINDER [METRES] ........- ')
      READ(*,1008)TANKL
      WRITE(*,1016) TANKD,TANKL
1016  FORMAT('0',4X,
     +'TANK DIAMETER ... -',F8.2,/,5X,
     +'TANK LENGTH ..... -',F8.2,/,/)
      WRITE(*,1012)
      READ(*,1003)ICHK
      IF(ICHK.GT.0)GO TO 200
      VTANK=3.1415*TANKD*TANKD/4.*TANKL
      TANKH=0.0
      TANKW=0.0
      TANKP=0.0
      RETURN
C
C**   SPHERICAL TANK
C
23    WRITE(*,1017)
1017  FORMAT('0',/,/,15X,'** SPHERICAL TANK DIMENSIONS **',/,/,/,11X,
     +'ENTER TANK DIAMETER [METRES] ..............- ')
      READ(*,1008)TANKD
      WRITE(*,1018)
1018  FORMAT('0',10X,'ENTER DEPTH OF TANK BURIED IN GROUND .......- ')
      READ (*,1008)TANKP
      WRITE(*,1019)TANKD,TANKP
1019  FORMAT('0',4X,
     +'TANK DIAMETER ..... -',F8.2,/,5X,
     +'TANK PENETRATION ... -',F8.2,/,/)
      WRITE(*,1012)
      READ(*,1003)ICHK
      IF(ICHK.GT.0)GO TO 200
```

```
      VTANK=4.18879*(TANKD/2)**3.
      TANKH=0.0
      TANKW=0.0
      TANKL=0.0
      RETURN
      END
      SUBROUTINE RUPTUR (IGAS)
      COMMON /RUPT/ IRUPT,HOLEH,RUPTA,CD,RUPTD,RUPTH,RUPTW,TOH,BOH
100   CONTINUE
C
C**  CLEAR SCREEN AND HOME CURSOR
C
      WRITE(*,1000)
1000  FORMAT('0',9(/,15X),'* * *  RUPTURE TYPE SELECTION MENU * * *',/,/
     +,/,' ORIFICE SHAPE       EDGE CONDITION            ORIENTATION',/,/
     +,' CIRCULAR               SMOOTH                          - 1-',/
     +,' CIRCULAR        UNIFORM PETALS JAGGED IN               - 2-',/
     +,' CIRCULAR        RANDOM PETALS JAGGED IN                - 3-',/
     +,' CIRCULAR        UNIFORM PETALS JAGGED OUT              - 4-',/
     +,' RECTANGULAR            SMOOTH                HORIZONTAL - 5-',/
     +,' RECTANGULAR            SMOOTH                VERTICAL   - 6-',/
     +,' RECTANGULAR     UNIFORM PETALS JAGGED IN     HORIZONTAL - 7-',/
     +,' RECTANGULAR     UNIFORM PETALS JAGGED IN     VERTICAL   - 8-',/
     +,' RECTANGULAR     RANDOM PETALS JAGGED IN      HORIZONTAL - 9-',/
     +,' RECTANGULAR     RANDOM PETALS JAGGED IN      VERTICAL   -10-',/
     +,' RECTANGULAR     UNIFORM PETALS JAGGED OUT    HORIZONTAL -11-',/
     +,' RECTANGULAR     UNIFORM PETALS JAGGED OUT    VERTICAL   -12-',/
     +)
C
C
C
      WRITE(*,1001)
1001  FORMAT('0',5X,'SELECT PUNCTURE TYPE ( # then RETURN) ..... - ')
      READ(*,1002) IRUPT
1002  FORMAT(I3)
      GO TO 11
11    WRITE(*,1003)
1003  FORMAT('0',5X,'ENTER THE DISTANCE FROM THE HOLE CENTRE TO',/,6X,
     +'THE BOTTOM OF THE TANK (metres) ............ - ')
      READ(*,1004)HOLEH
1004  FORMAT(F15.5)
C
C  BRANCH TO RECT OR CIRC ROUTINES
C
      IF (IRUPT.GT.4) GO TO 200
      WRITE(*,1005)
1005  FORMAT('0',5X,'ENTER THE DIAMETER OF THE RUPTURE (metres) ..- ')
      READ(*,1004)RUPTD
      RUPTA=RUPTD*RUPTD*3.1415/4.0
      RUPTW=0.0
      RUPTH=0.0
      GO TO 300
200   WRITE(*,1006)
1006  FORMAT('0',5X,'ENTER VERTICAL HEIGHT OF RUPTURE (metres) ...- ')
      READ (*,1004)RUPTH
```

```
      WRITE(*,1007)
1007  FORMAT('0',5X,'ENTER WIDTH OF RUPTURE (metres) .............- ')
      READ(*,1004)RUPTW
      RUPTA=RUPTH*RUPTW
      RUPTD=RUPTH
300   WRITE(*,1008)
1008  FORMAT('0',10X,'** REVIEW YOUR INPUTS **',/,/)
      IF(IRUPT.GT.4)GO TO 400
      WRITE(*,1009)IRUPT,HOLEH,RUPTD
1009  FORMAT(10X,
     +'RUPTURE TYPE (#) ............- ',7X,I3,/,10X,
     +'DIST HOLE TO TANK BOTTOM ...- ',F10.2,/,10X,
     +'RUPTURE DIAMETER ............- ',F10.4,/,/,10X,
     +'IF ABOVE ENTRIES OK [return] OTHERWISE [enter - 9 ] ..- ')
      GO TO 500
400   WRITE(*,1011)IRUPT,HOLEH,RUPTH,RUPTW
1011  FORMAT('0',9X,
     +'RUPTURE TYPE (#) ..............- ',7X,I3,/,10X,
     +'DIST HOLE TO TANK BOTTOM ......- ',F10.2,/,10X,
     +'RUPTURE HEIGHT ................- ',F10.4,/,10X,
     +'RUPTURE WIDTH .................- ',F10.4,/,/,5X,
     +'IF ABOVE ENTRIES OK [return] OTHERWISE [enter - 9 ] ..- ')
500   READ(*,1010)ICHK
1010  FORMAT(I2)
      IF(ICHK.GT.0) GO TO 100
      TOH=HOLEH+RUPTD/2
      BOH=HOLEH-RUPTD/2
      IF(IRUPT.GT.4)RUPTD=0.0
      IF(IGAS.GT.0)GO TO 600
C
C**  ASSIGN CD VALUE BASED ON PUNCTURE TYPE
C
      GO TO (101,102,103,104,105,106,107,108,109,110,111,112),IRUPT
101   CD=0.65
      GO TO 600
102   CD=0.622
      GO TO 600
103   CD=0.577
      GO TO 600
104   CD=0.619
      GO TO 600
105   CD=0.625
      GO TO 600
106   CD=0.624
      GO TO 600
107   CD=0.629
      GO TO 600
108   CD=0.626
      GO TO 600
109   CD=0.609
      GO TO 600
110   CD=0.613
      GO TO 600
111   CD=0.826
      GO TO 600
```

```
112       CD=0.828
          GO TO 600
600       IF (IGAS.GT.0)CD=0.61
          RETURN
          END
          SUBROUTINE INIT(TEMPT)
        COMMON /EQNS/CMASS,DLIQ,VLIQ,HLIQ,PT,VAPD,VAPP,HCAPG,RK,HCAPL,DHV
       +,VLIQI
          COMMON /CPROP/ TBOIL,TCRIT,PCRIT,RMW,A,B,C,IGAS,ICHEM
          COMMON /ENV/ TAIR,PATM,WINDS
          COMMON /TANK/ ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK,WALLT,
       +TINS,AINSD
          COMMON /RUPT/ IRUPT,HOLEH,RUPTA,CD,RUPTD,RUPTH,RUPTW,TOH,BOH
100       CONTINUE
C
C*** CLEAR SCREEN AND HOME CURSOR
C
          WRITE(*,1000)
1000      FORMAT('0',9X,'ENTER MASS OF CHEMICAL IN TANK (kg) ........- ')
          READ(*,1001)CMASS
1001      FORMAT(F12.1)
          WRITE(*,1002)CMASS
1002      FORMAT('0',9X,'MASS OF CHEMICAL INPUT WAS ..................- '
       +,F12.1,/,/,/,10X,'IF CORRECT [return] OTHERWISE [enter - 9 ] ..- '
       +)
          READ (*,1003)ICHK
1003      FORMAT(I2)
          IF(ICHK.GT.0)GO TO 100
          IF(IGAS.GT.0)GO TO 200
C
C** CLEAR SCREEN
C
          WRITE (1,1004)
1004      FORMAT('0',13X,'* * INITIAL CONDITIONS **',/,/,/)
C
C**  LIQUID
C
          ICALL=1
          CALL LEQNS(TEMPT,ICALL)
          VLIQI=VLIQ
          WRITE (1,1005)ICHEM,CMASS,TEMPT,DLIQ,VLIQ,HLIQ,PT,VAPD,VAPP,
       +HCAPG,RK,HCAPL,DHV
1005      FORMAT('0',
       +4X,'CHEMICAL TYPE CODE ..... - ',17X,I3,/,
       +5X,'MASS OF CHEMICAL (KG)..... - ',F20.8,/,
       +5X,'TEMP OF TANK (DEG K)..... - ',F20.8,/,
       +5X,'DENSITY OF LIQUID (KG/CU M)... - ',F20.8,/,
       +5X,'VOLUME OF LIQUID (CU M)..... - ',F20.8,/,
       +5X,'HEIGHT OF LIQUID (M)..... - ',F20.8,/,
       +5X,'TANK PRESSURE (N/SQ M)..... - ',F20.8,/,
       +5X,'VAPOUR DENSITY (KG/CU M)..... - ',F20.8,/,
       +5X,'VAPOUR PRESSURE (N/SQ M)..... - ',F20.8,/,
       +5X,'HEAT CAP GAS (J/KG*DEG K)..... - ',F20.8,/,
       +5X,'K ..... - ',F20.8,/,
       +5X,'HEAT CAP LIQUID (J/KG*DEG K).. - ',F20.8,/,
```

```
     +5X,'HEAT OF VAPOURIZATION (J/SEC). - ',F20.8,/)
        GO TO 300
C
C** GAS ROUTINE
C
200     ICALL=1
        CALL GEQNS(TEMPT,ICALL)
        WRITE(1,1006) ICHEM,CMASS,TEMPT,PT,VAPD,HCAPG,RK
1006    FORMAT('0',
     +4X,'CHEMICAL TYPE CODE ..... - ',18X,I2,/,
     +5X,'MASS OF CHEMICAL (KG)..... - ',F20.8,/,
     +5X,'TEMP OF TANK (DEG K)..... - ',F20.8,/,
     +5X,'TANK PRESSURE (N/SQ M..... - ',F20.8,/,
     +5X,'VAPOUR DENSITY (KG/CU M)... - ',F20.8,/,
     +5X,'HEAT CAP GAS (J/KG*DEG K).. - ',F20.8,/,
     +5X,'K ..... - ',F20.8,/,/,/)
300     WRITE(1,1010) TBOIL,TCRIT,PCRIT,RMW,A,B,C,IGAS,TAIR,PATM,
     +WINDS
        WRITE(1,9010) ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK
     WALLT,TINS,AINSD
        WRITE(1,9011) IRUPT,HOLEH,RUPTD,RUPTH,RUPTW,CD,RUPTA
1010    FORMAT(5X,'TBOIL ..... - ',F20.8,/
     +5X,'CRITICAL TEMPERATURE ... - ',F20.8,/
     +5X,'CRITICAL PRESSURE ..... - ',F20.8,/
     +5X,'MOLECULAR WEIGHT ..... - ',F20.8,/
     +5X,'A ..... - ',F20.8,/
     +5X,'B ..... - ',F20.8,/
     +5X,'C ..... - ',F20.8,/
     +5X,'IGAS ..... - ',17X,I3,/
     +5X,'AIR TEMPERATURE ..... - ',F20.8,/
     +5X,'ATMOSPHERIC PRESSURE ... - ',F20.8,/
     +5X,'WIND SPEED ..... - ',F20.8,/,/)
9010    FORMAT(5X,'TYPE OF TANK ..... - ',17X,I3,/
     +5X,'TANK LENGTH ..... - ',F20.8,/
     +5X,'TANK HEIGHT ..... - ',F20.8,/
     +5X,'TANK WIDTH ..... - ',F20.8,/
     +5X,'TANK DIAMETER..... - ',F20.8,/
     +5X,'TANK PENETRATION ..... - ',F20.8,/
     +5X,'VOLUME OF TANK ..... - ',F20.8,/
     +5X,'WALL THICKNESS OF TANK.. - ',F20.8,/
     +5X,'INSULATION THICKNESS.... - ',F20.8,/
     +5X,'AREA OF INSULATION LOST. - ',F20.8,/,/)
9011    FORMAT(5X,'RUPTURE TYPE ..... - ',17X,I3,/
     +5X,'HEIGHT OF RUP ABOVE GRD. - ',F20.8,/
     +5X,'RUPTURE DIAMETER..... - ',F20.8,/
     +5X,'RUPTURE HEIGHT..... - ',F20.8,/
     +5X,'RUPTURE WIDTH..... - ',F20.8,/
     +5X,'CD ..... - ',F20.8,/
     +5X,'RUPTURE AREA..... - ',F20.8,/,/,/)
        RETURN
        END
        SUBROUTINE LEQNS(TEMPT,ICALL)
        COMMON /CPROP/ TBOIL,TCRIT,PCRIT,RMW,A,B,C,IGAS,ICHEM
     COMMON /EQNS/CMASS,DLIQ,VLIQ,HLIQ,PT,VAPD,VAPP,HCAPG,RK,HCAPL,DHV
    +,VLIQI
```

```
      COMMON /TANK/ ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK,WALLT,
     +TINS,AINSD
      COMMON /ENV/ TAIR,PATM,WINDS
C
      R=8314.0
      TBC=TBOIL/TCRIT
      TR=TEMPT/TCRIT
C
C **     LIQUID DENSITY CALCULATIONS
C
      AA=1.39644-24.07*TR+102.615*TR*TR-255.719*TR**3.+355.805*TR**4.-
     +256.671*TR**5.+75.1088*TR**6.
      BB=13.4412-135.7437*TR+533.38*TR*TR-1091.453*TR**3.+1231.43*TR**
     +4.-728.227*TR**5.+176.737*TR**6.
      WW=3./7.*(TBC/(1-TBC))*ALOG10(PCRIT/101000.)-1.0
C
C
      DLIQ=(RMW*PCRIT)/(R*TEMPT*EXP(AA+WW*BB))
C
C ****   CALC VOL OF LIQUID AND LIQUID LEVEL IN TANK
C
      VLIQ=CMASS/DLIQ
      HLIQ=HEIGHT(VLIQ)
C
C ***  CALCULATE VAPOUR PRESSURE OF LIQUID & CHECK WITH TANK PRESSURE
C
      BD=36./TR-35.-TR**6.+42.*ALOG(TR)
      ALPHAC=0.9076*(1+(TBC*(ALOG(PCRIT/101000.))/(1-TBC)))
C
     VAPP=PCRIT/(10.**((0.118*BD)-(7.*ALOG10(TR))+(ALPHAC-7.)*(0.0364*
     +BD-ALOG10(TR))))
      IF(ICALL .NE. 1) GO TO 55
      IF(VAPP.GE.PATM)PT=VAPP
      IF(VAPP.LT.PATM)PT=PATM
55    CONTINUE
C
C******
C
C  ***  CALCULATE VAPOUR DENSITY
C
      CHCK=0.001
      DA=0.4278*R*R*TCRIT**(5./2.)/PCRIT
      DB=0.0867*R*TCRIT/PCRIT
      VBAR=R*TEMPT/PT
C
2     Z=(1./(1.-DB/VBAR))-(DA/(R*TEMPT**(3./2.)*VBAR*(1+DB/VBAR)))
      VBAR2=Z*R*TEMPT/PT
      CHCK2=VBAR2/VBAR
C
C****
      IF(CHCK2.LT.CHCK)GO TO 100
      IF(CHCK2.GE.0.99)GO TO 1
      CHCK=CHCK2
      VBAR=VBAR2
      GO TO 2
```

```
C
1       VAPD=RMW/VBAR2
C
        GO TO 3
100     WRITE(*,3000)
3000    FORMAT('0',/,/,/,/,/,10X,'***** ITERATIONS IN VAPOUR DENSITY ROUTI
     +NE ARE NOT CONVERGING ****** ',/,/)
        PAUSE
3       CONTINUE
C
C****  CALCULATE HEAT CAPACITIES
C
        HCAPG=4184./RMW*(A+B*TEMPT+C*TEMPT*TEMPT)
C
        PR=PT/PCRIT
C
C*** ISOTHERMAL PRESSURE CORRECTION TO Cp BY CURVE FROM PERRY'S
C
        DCP=((TR/1.686)**(0-3.72))*PR**.9155
        HCAPG=HCAPG+DCP*4184./RMW
C ****
C
        RK=HCAPG/(HCAPG-(8314.0/RMW))
C
        HCAPL=HCAPG+46860./RMW
C
C **** CALCULATE HEAT OF VAPOURIZATION
C
        DHVB=4184.0*TBOIL*(5.0*ALOG10(PCRIT/101000.)-2.17)
        DHVB=DHVB/(RMW*(.930-TBC))
C
C**   DHV IS THE HEAT OF EVAP
C
        DHV=DHVB*((1-TR)/(1-TBC))**0.38
C
C
        RETURN
        END
C
C *** FUNC SUBROUTINE TO DETERMINE LIQ LEVEL IN TANKS
C
        FUNCTION HEIGHT(VLIQ)
        COMMON /TANK/ ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK,WALLT,
     +TINS,AINSD
        TANKR=TANKD/2
        GO TO (11,12,13,14),ITANK
C *** RECT
11      HEIGHT=VLIQ/(TANKL*TANKW)
        RETURN
C *** HORIZONTAL CYLINDER
12      DUM1=VLIQ/TANKL
        TRR=TANKR*TANKR
C ** SELECT INITIAL HEIGHT
        IF(VLIQ .LT. VTANK/2)GO TO 7
C
```

```
C        TANK GREATER THAN HALF FULL
C
         HCLIQ=TANKR
1        THETA=(HCLIQ-TANKR)/TANKR
         DDD=2.*ARCOS(THETA)
         DUM2=TRR*3.1415-((TRR)/2.*(DDD-SIN(DDD)))
         IF(DUM2/DUM1 .GT. .99) GO TO 5
         HCLIQ=HCLIQ+(DUM1-DUM2)/(TRR*3.1415)
         GO TO 1
C #### TANK LESS THAN HALF FULL
7        HCLIQ=0.0
2        THETA=(TANKR-HCLIQ)/TANKR
         DDD=2.*ARCOS(THETA)
         DUM2=TRR/2.*(DDD-SIN(DDD))
         IF(DUM2/DUM1 .GT. .99) GO TO 5
         HCLIQ=HCLIQ+(DUM1-DUM2)/(TRR*3.1415)
         GO TO 2
5        HEIGHT=HCLIQ
         RETURN
C *** VERTICAL CYLINDER
13       HEIGHT=VLIQ/(TANKR*TANKR*3.1415)
         RETURN
C ***  SPHERICAL TANK
14       VFRACT=3.*VLIQ/(4.*3.1415*TANKR**3)
         IF (VFRACT.GT..001)GO TO 10
         HEIGHT=0.0
         RETURN
10       IF(VFRACT.LT.0.999) GO TO 20
         HEIGHT=2.*TANKR
         RETURN
20       X=2.*VFRACT
                 DO 30 IK=1,6
                 F=X**3-3*X*X+4*VFRACT
                 FF=3.*X*X-6.*X
                 X=X-F/FF
30               CONTINUE
         HEIGHT=X*TANKR
         RETURN
         END
C
C ** INVERSE SINE FUNCTION
C
         FUNCTION ARCOS(THETA)
         ARCOS=3.1415927/2.-(THETA+THETA**3/6.+THETA**5*3./40.+THETA**7*5
     +./112.)
         RETURN
         END
         SUBROUTINE GEQNS(TEMPT,ICALL)
         COMMON /CPROP/ TBOIL,TCRIT,PCRIT,RMW,A,B,C,IGAS,ICHEM
       COMMON /EQNS/CMASS,DLIQ,VLIQ,HLIQ,PT,VAPD,VAPP,HCAPG,RK,HCAPL,DHV
     +,VLIQI
         COMMON /TANK/ ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK,WALLT,
     +TINS,AINSD
C
         R=8314.0
```

```
      TBC=TBOIL/TCRIT
      TR=TEMPT/TCRIT
      DA=0.4278*R*R*TCRIT**(5./2.)/PCRIT
      DB=0.0867*R*TCRIT/PCRIT
      IF(ICALL.EQ.2) GO TO 5
C
C *** CALCULATE TANK PRESSURE
C
      VBAR=VTANK*RMW/CMASS
      Z=1./(1.-DB/VBAR)-DA/(R*TEMPT**(3./2.)*VBAR*(1+DB/VBAR))
      PT=Z*R*TEMPT/VBAR
      GO TO 4
C
C  ***  CALCULATE VAPOUR DENSITY
C
5     CHCK=0
      VBAR=R*TEMPT/PT
C
2     Z=1./(1.-DB/VBAR)-DA/(R*TEMPT**(3./2.)*VBAR*(1+DB/VBAR))
      VBAR2=Z*R*TEMPT/PT
      CHCK2=VBAR2/VBAR
      IF(CHCK2.LT.CHCK)GO TO 100
      IF(CHCK2.GE.0.99)GO TO 1
      CHCK=CHCK2
      VBAR=VBAR2
      GO TO 2
C
1     VAPD=RMW/VBAR2
C
      GO TO 3
100   WRITE(*,3000)
3000  FORMAT('0',/,/,/,/,/,10X,'***** ITERATIONS IN VAPOUR DENSITY ROUTI
     +NE ARE NOT CONVERGING ****** ',/,/)
      PAUSE
4     VAPD=CMASS/VTANK
3     CONTINUE
C
C****  CALCULATE HEAT CAPACITIES
C
      HCAPG=4184./RMW*(A+B*TEMPT+C*TEMPT*TEMPT)
C
      PR=PT/PCRIT
C
C*** ISOTHERMAL PRESSURE CORRECTION TO Cp BY CURVE FROM PERRY'S
C
      DCP=((TR/1.686)**(0-3.72))*PR**.9155
20    HCAPG=HCAPG+DCP*4184/RMW
C
      RK=HCAPG/(HCAPG-(8314.0/RMW))
C
C
      RETURN
      END
      SUBROUTINE TEMP(DTIME,ME,TEMPT)
      REAL ME
```

```
      COMMON /ENV/ TAIR,PATM,WINDS
      COMMON /CPROP/ TBOIL,TCRIT,PCRIT,RMW,A,B,C,IGAS,ICHEM
     COMMON /EQNS/ CMASS,DLIQ,VLIQ,HLIQ,PT,VAPD,VAPP,HCAPG,RK,HCAPL,DHV
     +,VLIQI
      COMMON /TANK/ ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK,WALLT,
     +TINS,AINSD
      COMMON /MOD/ CTIME,EE,BETA,I,IJ,UO,HTAREA,JCALL,K
C
C
      IF (TEMPT .EQ. TAIR) GO TO 400
      RKI=0.00274
      RKW=16.45
C
C ** GET HEAT TRANSFER COEFF FOR DIFF TANK CONFIGURATIONS
C
      GO TO (1,2,2,3), ITANK
1     DC=0.104
      RM=0.675
      RL=AMIN1(TANKL,TANKW,TANKH)
      GO TO 100
2     DC=0.0266
      RM=0.805
      RL=TANKD
      GO TO 100
3     DC=0.06
      RM=0.50
      RL=TANKD
100   HO=0.017*DC/RL*(66700.*RL*WINDS)**RM
C
C** FUNCTION SUB TO CALC HEAT TRANSFER AREAS
C
      HTAREA=XHTA(HLIQ)
C ** CHECK TO SEE IF TANK IS INSULATED
      IF(TINS .EQ. 0.0) GO TO 200
      HI=1
C ** FOR INSULATED TANKS CALC UO DIRECTLY
C
150   UO=1/(1/HI+WALLT/RKW+TINS/RKI+1/HO)
C ** IF ANY INSULATION IS MISSING BRANCH TO ROUTINE TO ADJUST UO
C
      IF(AINSD.GT.0.0) GO TO 300
C
C ** CALCULATED NEW TANK TEMP
C
175   BUM1=ME*DHV*DTIME
      BUM2=UO*HTAREA*DTIME*(TAIR-TEMPT)
      BUM3=DLIQ*VLIQ*HCAPL
      TEMPT=TEMPT-(BUM1-BUM2)/BUM3
      RETURN
C
C** CHECK TO SEE IF TEMPT < TBOIL : HI CAN THEN BE CALC DIRECTLY
C
200   IF(TEMPT .LT. TBOIL) GO TO 300
      RP=VAPP/PCRIT
      HI=3.0E-06*PCRIT**1.69*RP**0.35*(1-RP)**0.9*(1.8*RP**0.17+4*RP**
```

```
     +1.2+10*RP**10.)
        GO TO 150
C
C ** CALC HI FOR TEMPT > TBOIL
C
C ** ASSUME TWALL = (TEMPT + TAIR)/2  AS A FIRST GUESS
C
300     DTEMP=(TAIR-TEMPT)/2
310     HI=69*DTEMP**0.25/HLIQ**0.25
        UOO=1/(1/HI+WALLT/RKW+1/HO)
        DTDUM=UOO/HI*(TAIR-TEMPT)
456     FORMAT(5X,5(F20.5,/))
        DUM=DTEMP/DTDUM
C
C ** CHECK FOR CONVERGENCE ie CORRECT  TWALL
C
        IF(DUM .GT. 0.975 .AND. DUM .LT. 1.025) GO TO 315
        DTEMP=DTDUM
        GO TO 310
315     IF(TINS .EQ. 0.0) GO TO 325
        UO=UO*(1-AINSD/HTAREA)+UOO*(AINSD/HTAREA)
        GO TO 175
325     UO=UOO
        GO TO 175
400     RETURN
        END
        FUNCTION XHTA(HLIQ)
        COMMON /TANK/ ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK,WALLT,
     +TINS,AINSD
C *** THIS ROUTINE CALCULATES THE TANK WALL AREA FOR HEAT TRANSFER
C
        TANKR=TANKD/2.
        GO TO (1,2,3,4),ITANK
1       XHTA=2.0*HLIQ*(TANKL+TANKW)+TANKL*TANKW
        RETURN
2       THETA=(TANKR-HLIQ)/TANKR
        XHTA=2*TANKR*ARCOS(THETA)*TANKL
        RETURN
3       XHTA=3.1415*TANKD*TANKD/4.+3.1415*TANKD*HLIQ
        RETURN
4       XHTA=6.2832*TANKR*(HLIQ-TANKP)
        RETURN
        END
        SUBROUTINE LIQMOD(TEMPT,ITPF)
        REAL MASSFR,MESAT,ME
        COMMON /CPROP/ TBOIL,TCRIT,PCRIT,RMW,A,B,C,IGAS,ICHEM
        COMMON /ENV/ TAIR,PATM,WINDS
        COMMON /TANK/ ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK,WALLT,
     +TINS,AINSD
        COMMON /RUPT/ IRUPT,HOLEH,RUPTA,CD,RUPTD,RUPTH,RUPTW,TOH,BOH
      COMMON /EQNS/ CMASS,DLIQ,VLIQ,HLIQ,PT,VAPD,VAPP,HCAPG,RK,HCAPL,DHV
     +,VLIQI
        COMMON /MOD/CTIME,EE,BETA,I,IJ,UO,HTAREA,JCALL,K
C
        WRITE(*,789)
```

```
789     FORMAT('0',10X,'* *   LIQUID MODEL   **',/)
        WRITE(1,123)
123     FORMAT('1')
        MLL=0
        IJ=1
        ICALL=2
        JCALL=1
        R=8314.
        TBUBV=0
C
C** CALCULATE BETA
C
        IF(IRUPT.GT.4) RUPTD=(RUPTH*RUPTW)**.5
        IF(ITANK.EQ.1) TANKD=(TANKW*TANKL*TANKH)**.3333
        BETA=RUPTD/TANKD
C
C** CHANGE IN LIQ LEVEL FOR EACH ITERATION SET AT 5 CM
        DH=.05
C
C ** INIT PRESSURE CONDITION IN TANK ESTABLISHED IN FIRST CALL OF INIT
C
C
C ** MAIN LOOP IN OUTFLOW ROUTINE
C
1       GO TO 3
2       PT=PATM
3       CONTINUE
        PTO=(HLIQ-HOLEH+RUPTD/2)*DLIQ*9.81+PT
5       IF(PTO.GE.(1.01*PATM).OR. MLL.EQ.1) GO TO 10
C
C ** AIR INGESTION ROUTINE
C
        BUBV=(1.01*PATM-PTO)*(VTANK-VLIQ)*TAIR/(PATM*TEMPT)
        TBUBV=TBUBV+BUBV
        DPRESS=PATM*(TEMPT/TAIR)*(BUBV/(VTANK-VLIQ))
        PT=PT+DPRESS
        IF(PT.GT.PATM)PT=PATM
        PTO=1.01*PATM
C
C
C ** IF TPF CHECK FOR SONIC/SUBSONIC FLOW
C ** IF JUST LIQ FLOW BRANCH TO SIMPLE MASSFR EQN
C ** CALC STAGNATION QUALITY AND CRIT PRESS RATIO
C
10      IF (ITPF .EQ. 0) GO TO 9
        XO=VAPD/(VAPD+((1/EE)-1)+DLIQ)
        CPR=EXP(0.0-.4353*XO-0.1625)
        PR=PATM/PTO
        IF(PR.LE.CPR)GO TO 111
C ** MASSFR FOR SUB-SONIC CONDITIONS & TPF
        Y=1-((1-PR)/RK)*(0.41+0.35*BETA**4.)
        IF(XO.EQ.0.) Y=1
        DUM1=CD*RUPTA*Y/(SQRT(1-BETA**4.))
        DUM2=SQRT(2*(PTO-PATM)/(XO**1.5*(1/VAPD-1/DLIQ)+1/DLIQ))
        MASSFR=DUM1*DUM2
```

```
        GO TO 222
C ** MASSFR FOR SONIC CONDITIONS & TPF
111     DUM1=CD*RUPTA/(SQRT(1-BETA**4.))
        DUM2=(1-EE)/EE
      DUM3=2*DLIQ*PTO*(1-EE)*DUM2*(1-CPR)+RK/(RK-1)*(1-CPR**((RK-1)/RK))
        DUM4=(1-XO)*EE*(DUM2+CPR**(-1./RK))**2.
        MASSFR=SQRT(DUM3/DUM4)
        GO TO 222
9       MASSFR=(CD*RUPTA*(2*(PTO-PATM)*DLIQ)**.5)/SQRT(1-BETA**4.)
222     MESAT=VAPD*MASSFR/(DLIQ-VAPD)
        SACHEM=ASC(HLIQ)
        ME=MESAT-(1.9*MESAT**(5./4.))/(DLIQ*SACHEM*SQRT(R*TEMPT))**.25
        OVLIQ=VLIQ
        HLIQ=HLIQ-DH
        IF (HLIQ .GT. 0) GO TO 543
        HLIQ=0
        VLIQ=0
        GO TO 6
543     RHLIQ=HLIQ
        VLIQ=VOL(DH,HLIQ,SACHEM)
        DVOL=OVLIQ-VLIQ
C ***
        IF (ITPF .EQ. 1 ) GO TO 333
        PT=PT*(VTANK-OVLIQ)/(VTANK-VLIQ)
        IF(PT.LT.VAPP)PT=VAPP
        GO TO 444
C ***   PRESSURE ADJUSTMENT FOR TPF SITUATION
333     PT=VAPP
444     CMASS=VLIQ*DLIQ
        DTIME=DLIQ*DVOL/(ME+MASSFR)
        CTIME=CTIME+DTIME
C ** TEMP DROP DUE TO EVAPORATION
        DTEV=ME*DHV*DTIME/(VLIQ*DLIQ*HCAPL)
        TEMPT=TEMPT-DTEV
        IF(VAPP.GT.PATM.AND.TEMPT.LT.TBOIL)TEMPT=TBOIL
C
C** CALL TEMP ROUTINE HERE : BRINGS TEMP BACK UP BY HEAT TRANSFER
C
        CALL TEMP(DTIME,ME,TEMPT)
        TEMPT=TEMPT+DTEV
        CALL LEQNS(TEMPT,ICALL)
C
C ** CHECK FOR TWO PHASE FLOW
        IF(VAPP.GT.PATM) GO TO 12
        ITPF=0
        GO TO 14
12      EE=EPSIL(ME,SACHEM,TANKD,TEMPT)
        EEMAX=(VTANK-VLIQ)/VTANK
        IF(EE.GT.EEMAX) EE=EEMAX
        IF(EE.LE..01) ITPF=0
        IF(EE.GT..01) ITPF=1
C
C** OUTPUT INFO EVERY 50 STEPS AND AT TOP AND BOTTOM OF HOLE
C
        IF(ITPF.EQ.0) GO TO 14
```

```
          VOLX=VLIQ/(1-EE)
          RHLIQ=HEIGHT(VOLX)
 14       IF(VLIQ.GT.(VLIQI*I/10)) GO TO 15
          I=I-1
 7        WRITE(1,1000)VLIQ,CTIME,DVOL,DTIME,DLIQ,HLIQ,VAPP,VAPD,HCAPG,
     +HCAPL,RK,DHV,TBUBV,TEMPT,PT
 1000     FORMAT('0',4X,
     +'VOLUME OF LIQUID IN TANK ....- ',F20.6,/,5X
     +'ELAPSED TIME .................- ',F20.6,/,5X
     +'LOSS OF LIQ. EACH ITERATION .- ',F20.6,/,5X
     +'TIME FOR LAST ITERATION .....- ',F20.6,/,5X
     +'LIQUID DENSITY ..............- ',F20.6,/,5X
     +'HEIGHT OF LIQUID ............- ',F20.6,/,5X
     +'VAPOUR PRESSURE .............- ',F20.6,/,5X
     +'DENSITY OF VAPOUR ...........- ',F20.6,/,5X
     +'HEAT CAPACITY OF VAPOUR .....- ',F20.6,/,5X
     +'HEAT CAPACITY OF LIQUID .....- ',F20.6,/,5X
     +'K ............................- ',F20.6,/,5X
     +'HEAT OF VAPOURIZATION .......- ',F20.6,/,5X
     +'TOTAL VOL OF AIR INGESTED ...- ',F20.6,/,5X
     +'TEMPERATURE IN TANK .........- ',F20.6,/,5X
     +'PRESSURE IN TANK ............- ',F20.6,/,5X)
          IF (ITPF .EQ. 0) GO TO 234
          WRITE(1,1001)XO,EE,RHLIQ
 1001     FORMAT('+',4X,
     +'STAGNATION QUALITY ..........- ',F20.6,/,5X,
     +'EPSILON - VAPOUR VOID FRAC ..- ',F20.6,/,5X,
     +'HEIGHT OF BOILING LIQUID ....- ',F20.6)
C ** EJECT PAGE CHECK
 234      WRITE(1,1002)
 1002     FORMAT('0')
          IF (IJ .LT. 3) GO TO 11
          WRITE (1,123)
          IJ=0
 11       IJ=IJ+1
          IF(K.EQ.2)GO TO 8
 15       CONTINUE
          IF (HLIQ.GE.TOH.OR.RHLIQ.GE.TOH)GO TO 1
C ** CONTINUE OUTFLOW BELOW TOP OF HOLE
 357      FORMAT(4X,'GOT TO',I3)
          MLL=1
          IF(HLIQ.GT.BOH.AND.VAPP.LT.PATM)GO TO 2
          IF(HLIQ.GT.BOH.AND.VAPP.GE.PATM)GO TO 1
          IF(VAPP.GT.PATM) GO TO 66
          JCALL=99
          GO TO 6
 66       IF(VLIQ.GT.0.0) CALL VAPMOD(TEMPT,JCALL)
          WRITE(*,507)
 507      FORMAT(3X,'BACK IN LIQUID MODEL')
          IF(JCALL.NE.99) GO TO 1
          RETURN
 6        K=2
          GO TO 7
 8        RETURN
          END
```

```
C
C***  FUNCTION SUBPROG TO DETERMINE SURFACE AREA OF LIQUID IN TANK
C
        FUNCTION ASC(HLIQ)
        COMMON /TANK/ ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK,WALLT,
     +TINS,AINSD
        TANKR=TANKD/2
        GO TO (1,2,3,4),ITANK
C ** RECTANGULAR
1       ASC=TANKW*TANKL
        RETURN
C** UPRIGHT CYLINDER
3       ASC=3.1415*TANKR*TANKR
        RETURN
C** HORIZONTAL CYLINDER
2       THETA=(TANKR-HLIQ)/TANKR
        ASC=TANKL*2.*TANKR*SIN(ARCOS(THETA))
        RETURN
C** SPHERICAL
4       ASC=3.1415*(2.*HLIQ*TANKR-HLIQ*HLIQ)
        RETURN
        END
C
C ** FUNC SUBPROG TO CALC VOL OF LIQ IN TANK GIVEN LIQ LEVEL
C
        FUNCTION VOL(DH,HLIQ,SACHEM)
        COMMON /TANK/ ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK,WALLT,
     +TINS,AINSD
        TANKR=TANKD/2.
        GO TO (1,2,1,4),ITANK
C ** FOR RECTANGULAR TANKS & VERTICAL CYLINDERS (UNIFORM X-SECTION)
1       VOL=HLIQ*SACHEM
        RETURN
2       THETA=(TANKR-HLIQ)/TANKR
        DDD=2*ARCOS(THETA)
        VOL=TANKL*TANKR*TANKR/2*(DDD-SIN(DDD))
        RETURN
4       VOL=1.04719*HLIQ*HLIQ*(3*TANKR-HLIQ)
        RETURN
        END
C
C ** FUNC SUBPROG TO CALCULATE VOID FRACTION THAT'S VAPOUR (EPSILON)
C
        FUNCTION EPSIL(ME,SACHEM,TANKD,TEMPT)
        REAL ME
      COMMON /EQNS/ CMASS,DLIQ,VLIQ,HLIQ,PT,VAPD,VAPP,HCAPG,RK,HCAPL,DHV
     +,VLIQI
        COMMON /CPROP/ TBOIL,TCRIT,PCRIT,RMW,A,B,C,IGAS,ICHEM
        UOG=ME/(VAPD*SACHEM)
        SIGMA=6.56E-07*DHV*DLIQ
        DUM=SQRT(SIGMA/(9.81*(DLIQ-VAPD)))
        DUM2=37.*CMASS**.1666*VAPD*(TEMPT+1.47*TBOIL)/(DLIQ**1.1666*TEMP
     +T**1.5)
        EPSIL=0.73*(UOG*UOG/(9.81*DUM))**0.376*(DUM/TANKD)**0.176*(DLIQ/
     +(DLIQ-VAPD))**0.585*DUM2**0.256
```

```
      RETURN
      END
CCCCC
CCCCC
      SUBROUTINE GASMOD(TEMPT)
      REAL MASS2,MASSO,MASSFR
      COMMON /CPROP/ TBOIL,TCRIT,PCRIT,RMW,A,B,C,IGAS,ICHEM
      COMMON /ENV/ TAIR,PATM,WINDS
      COMMON /TANK/ ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK,WALLT,
     +TINS,AINSD
      COMMON /RUPT/ IRUPT,HOLEH,RUPTA,CD,RUPTD,RUPTH,RUPTW,TOH,BOH
      COMMON /EQNS/ CMASS,DLIQ,VLIQ,HLIQ,PT,VAPD,VAPP,HCAPG,RK,HCAPL,DHV
     +,VLIQI
      COMMON /MOD/CTIME,EE,BETA,I,IJ,UO,HTAREA,JCALL,K
C
C
      WRITE(1,222)
222   FORMAT('1')
      WRITE (1,678)
678   FORMAT(5X,' * *   GAS MODEL   * *',/)
      I=1
      J=1
      ICALL=2
C
C ** CHECK FOR SONIC FLOW
C
      IF(IRUPT.GT.4)RUPTD=(RUPTH*RUPTW)**.5
      IF(ITANK.EQ.1)TANKD=(TANKW*TANKL*TANKH)**.3333
      BETA=RUPTD/TANKD
      IF(BETA.LE..2)GO TO 1
      WRITE(*,99)BETA
99    FORMAT('0',9(/,5X,),'* * BETA GREATER THAN 0.2 * * - BETA = ',
     +F6.2,/,/)
      PAUSE
1     CPR=(2/(RK+1))**(RK/(RK-1))
C
C ****
C
      PAT=PATM/PT
      IF(CPR.LT.PAT) GO TO 100
C
C ** SONIC FLOW  20 ITERATIONS IN PRESSURE  DPRESS
C
      II=0
      DPRESS=(PT-(PATM/CPR))/20.
      DO 1000 I=1,20,1
      II=II+1
C
      MASSFR=CD*RUPTA*(RK*(PT*VAPD)*((2/(RK+1))**((RK+1)/(RK-1))))**.5
      PT=PT-DPRESS
C ** DET VAPOUR DENSITY &K BY SUBPROGRAM GEQNS.FOR
      CALL GEQNS(TEMPT,ICALL)
      MASS2=VAPD*VTANK
      MASSO=CMASS-MASS2
      CMASS=MASS2
```

```
          TIME=MASSO/MASSFR
          CTIME=CTIME+TIME
          IF(II.LT.10)GO TO 2
          WRITE(1,98)MASS2,MASSO,TIME,CTIME,PT,VAPD,HCAPG,RK
          II=0
98        FORMAT('0',4X,
         +' MASS REMAINING IN TANK ..... - ',F20.6,/,5X,
         +' MASS LOST IN EACH PRESSURE STEP ..- ',F20.6,/,5X,
         +' TIME TO LOSE MASS ..... - ',F20.6,/,5X,
         +' CUMULATIVE TIME ..... - ',F20.6,/,5X,
         +' PRESSURE IN TANK ..... - ',F20.6,/,5X,
         +' VAPOUR DENSITY ..... - ',F20.6,/,5X,
         +' HEAT CAPACITY OF GAS ..... - ',F20.6,/,5X,
         +' K ..... - ',F20.6,/,5X,/,/)
2         CONTINUE
1000      CONTINUE
          WRITE(1,222)
C
C *** SUB-SONIC FLOW  20 ITERATIONS IN D-PRESSURE
C
100       DPRESS=(PATM/CPR-PATM)/20.
          JJ=0
          DO 500 J=1,20,1
          JJ=JJ+1
          PAT=PATM/PT
          Y=1-(((1-PAT)/RK)*(0.41+0.35*BETA**4))
          MASSFR=CD*RUPTA*Y*((2.*(PT-PATM)*VAPD)**.5)/((1-BETA**4)**.5)
          PT=PT-DPRESS
C ** DET VAPOUR DENSITY & K BY SUBPROG
          CALL GEQNS(TEMPT,ICALL)
          MASS2=VAPD*VTANK
          MASSO=CMASS-MASS2
          CMASS=MASS2
          TIME=MASSO/MASSFR
          CTIME=CTIME+TIME
          IF(JJ.LT.5) GO TO 3
          WRITE(1,98)MASS2,MASSO,TIME,CTIME,PT,VAPD,HCAPG,RK
          JJ=0
3         CONTINUE
500       CONTINUE
          RETURN
          END
CCCCC
CCCCC
          SUBROUTINE VAPMOD(TEMPT)
          REAL ME,MASSFR,MESAT
          COMMON /CPROP/ TBOIL,TCRIT,PCRIT,RMW,A,B,C,IGAS,ICHEM
          COMMON /ENV/ TAIR,PATM,WINDS
          COMMON /TANK/ ITANK,TANKL,TANKH,TANKW,TANKD,TANKP,VTANK,WALLT,
        +TINS,AINSD
          COMMON /RUPT/ IRUPT,HOLEH,RUPTA,CD,RUPTD,RUPTH,RUPTW,TOH,BOH
         COMMON /EQNS/ CMASS,DLIQ,VLIQ,HLIQ,PT,VAPD,VAPP,HCAPG,RK,HCAPL,DHV
        +,VLIQI
          COMMON /MOD/CTIME,EE,BETA,I,IJ,UO,HTAREA,JCALL,K
          CDV=0.61
```

```
      IO=0
      IOP=1
      WRITE (*,678)
678   FORMAT('0','* *   VAPOUR MODEL   * *',/)
      R=8314.
      DH=.05
      DUMK=(RK+1)/(RK-1)
      DA=0.4278*R*R*TCRIT**(5/2)/PCRIT
      DB=0.0867*R*TCRIT/PCRIT
      ICALL=2
      IF (JCALL.NE.0) GO TO 500
C ** INITIALIZE CTIME;CALC BETA,TOH,BOH
      IF(IRUPT.GT.4)RUPTD=(RUPTH*RUPTW)**.5
      IF(ITANK.EQ.1) TANKD=(TANKW*TANKL*TANKH)**.3333
      BETA=RUPTD/TANKD
      TBUBV=0.0
      EE=0.0
      I=9
      IJ=1
      WRITE(1,777)
777   FORMAT('1')
500   CONTINUE
C** CALC INITIAL MASS OF CHEM IN VAPOUR SPACE
      VSMASS=(VTANK-VLIQ)*VAPD
C** CHECK FLOW REGIME AND BRANCH TO SONIC OR SUB-SONIC FLOW
      CPR=(2./(RK+1.))**(RK/(RK-1))
1000  PR=PATM/PT
      IF(PR .GT. CPR) GO TO 100
C ** SONIC
      MASSFR=CDV*RUPTA*SQRT(RK*PT*VAPD*(2/(RK+1))**DUMK)
      WRITE(*,441)
441   FORMAT(5X,'SONIC')
      GO TO 200
C ** SUB-SONIC
100   Y=1-((1-PR)/RK*(0.41+.35*BETA**4.))
      DUM=SQRT(1.-BETA**4.)
      MASSFR=CDV*RUPTA*Y/DUM*(2.*(PT-PATM)*VAPD)**.5
      WRITE(*,554)
554   FORMAT(5X,'SUB-SONIC')
200   SACHEM=ASC(HLIQ)
      WRITE(*,132)SACHEM,MASSFR,TANKD,TEMPT
132   FORMAT(5X,'SACHEM= ',F20.10,/,'MASSFR =',F20.10,/,
     +'TANKD =',F20.10,/,'TEMPT = ',F20.10,/)
      EEO=EE
      EE=EPSIL(MASSFR,SACHEM,TANKD,TEMPT)
      WRITE(*,139)EE
139   FORMAT(10X,'EE= ',F20.10,/,/)
C ** CHECK ACTUAL HEIGHT OF LIQUID IN TANK (FROTHING LIQ)
      VLIQX=VLIQ/(1-EE)
      RHLIQ=HEIGHT(VLIQX)
        EEMAX=(VTANK-VLIQ)/VTANK
      IF(EE.LE.EEMAX.AND. RHLIQ.LT.BOH) GO TO 502
      EE=EEMAX
      DEE=EE-EEO
      ITPF=1
```

```
      TEMPT=TEMPT-(DEE*VTANK*VAPD*DHV/(CMASS*HCAPL))
      IF(TEMPT.LT.TBOIL)TEMPT=TBOIL
      CALL LEQNS(TEMPT,ICALL)
      IF(VAPP.LT.PATM) VAPP=1.01*PATM
      PT=VAPP
      RETURN
502   XO=VAPD/(VAPD+((1/EE)-1)*DLIQ)
      MESAT=MASSFR
      ME=MESAT-(1.9*MESAT**(5/4))/(DLIQ*SACHEM*SQRT(R*TEMPT))**0.25
C
      IF(TEMPT.GT.TBOIL) GO TO 963
      ME=UO*HTAREA*(TAIR-TEMPT)/DHV
      DTIME=DLIQ*VLIQ/ME
      PT=PATM
      WRITE(1,135)VLIQ,DTIME
135   FORMAT('0',5X,'VOLUME OF LIQ WHEN TEMP TANK = TBOIL - ',F10.3,
     +/,5X,'TIME TO LOSE THIS REMAINING LIQUID   - ',F10.0)
      VLIQ=0
      HLIQ=0
400   CTIME=CTIME+DTIME
      JCALL=99
      RHLIQ=0
      K=2
      GO TO 7
C
963   OVLIQ=VLIQ
      HLIQ=HLIQ-DH
      IF(HLIQ .GT. 0)GO TO 300
      VLIQ=0.0
      HLIQ=0.0
      CMASS=VAPD*VTANK
      DVOL=OVLIQ-VLIQ
      DTIME=DLIQ*DVOL/ME
      GO TO 400
300   VLIQ=VOL(DH,HLIQ,SACHEM)
      DVOL=OVLIQ-VLIQ
      DTIME=DLIQ*DVOL/ME
      CTIME=CTIME+DTIME
C ** TEMPERATURE DROP DUE TO EVAPORATION
      DTEV=ME*DHV*DTIME/(VLIQ*DLIQ*HCAPL)
      TEMPT=TEMPT-DTEV
C     IF (TEMPT .LT. TBOIL) TEMPT=TBOIL
      CALL TEMP(DTIME,ME,TEMPT)
      TEMPT=TEMPT+DTEV
      CALL LEQNS(TEMPT,ICALL)
      IF(TEMPT.LE.TBOIL.OR.VAPP.LT.PATM)VAPP=1.01*PATM
C ** CALCULATE NEW TANK PRESSURE
      DVSMAS=(MASSFR-ME)*DTIME-DVOL*VAPD
      VSMASS=VSMASS-DVSMAS
      DVBAR=(VTANK-VLIQ)*RMW/DVSMAS
      Z=1/(1-DB/DVBAR)-DA/(R*TEMPT**(3/2)*DVBAR*(1+DB/DVBAR))
      PT=VAPP-(Z*R*TEMPT/DVBAR)
      IF (PT.LE.PATM)PT=1.01*PATM
      CMASS=CMASS-MASSFR*DTIME
C ** CHECK ACTUAL HEIGHT OF LIQUID IN TANK (FROTHING LIQ)
```

```
      VLIQX=VLIQ/(1-EE)
      RHLIQ=HEIGHT(VLIQX)
      IF(VLIQ .GT. (VLIQI*I/10)) GO TO 15
      I=I-1
7     WRITE(1,1011)VLIQ,CTIME,DVOL,DTIME,DLIQ,HLIQ,VAPP,VAPD,HCAPG,
     +HCAPL,RK,DHV,TEMPT,PT
1011  FORMAT('0',4X,
     +'VOLUME OF LIQUID IN TANK ....- ',F20.6,/,5X
     +'ELAPSED TIME ................- ',F20.6,/,5X
     +'LOSS OF LIQ. EACH ITERATION .- ',F20.6,/,5X
     +'TIME FOR LAST ITERATION .....- ',F20.6,/,5X
     +'LIQUID DENSITY ..............- ',F20.6,/,5X
     +'HEIGHT OF LIQUID ............- ',F20.6,/,5X
     +'VAPOUR PRESSURE .............- ',F20.6,/,5X
     +'DENSITY OF VAPOUR ...........- ',F20.6,/,5X
     +'HEAT CAPACITY OF VAPOUR .....- ',F20.6,/,5X
     +'HEAT CAPACITY OF LIQUID .....- ',F20.6,/,5X
     +'K ...........................- ',F20.6,/,5X
     +'HEAT OF VAPOURIZATION .......- ',F20.6,/,5X
     +'TEMPERATURE IN TANK .........- ',F20.6,/,5X
     +'PRESSURE IN TANK ............- ',F20.6,/,5X)
      WRITE(1,1001)XO,EE,RHLIQ
1001  FORMAT('+',4X,
     +'STAGNATION QUALITY ..........- ',F20.6,/,5X,
     +'EPSILON - VAPOUR VOID FRAC ..- ',F20.6,/,5X,
     +'HEIGHT OF BOILING LIQUID ....- ',F20.6)
C **  EJECT PAGE CHECK
      IF (IJ .LT. 3) GO TO 11
      WRITE (1,123)
123   FORMAT('1')
      IJ=0
11    IJ=IJ+1
      IF(K.EQ.2) GO TO 101
15    CONTINUE
      IF(RHLIQ.LT.TOH) GO TO 16
      K=2
      GO TO 7
16    IF(VLIQ.GT.0.0) GO TO 1000
      JCALL=99
      K=2
      GO TO 7
101   RETURN
      END
```